Operator Theory
Advances and Applications
276

Pavel Kurasov
Ari Laptev
Sergey Naboko
Barry Simon
Editors

Analysis as a Tool in Mathematical Physics

In Memory of Boris Pavlov

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In Memoriam

Boris Pavlov (1936–2016)
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Professor **Boris Pavlov** (**Борис Сергеевич Павлов**) passed away on January 30, 2016, just a few months before his 80th birthday. He was one of the brightest and most influential members of Leningrad/Saint Petersburg Mathematical School. In particular, he was the founder of the Leningrad school of non-self-adjoint operators. Born in Kronshtadt (an island in the Finish Gulf visible from Leningrad when the weather is good) on July 27, 1936, he entered the Physics Faculty of Leningrad University in 1953. His supervisor was M.S. Birman, an outstanding specialist in mathematical physics and operator theory. In fact, Pavlov was the first PhD student of the at-that-time young professor Birman. Boris Pavlov's thesis, devoted to the spectral theory of non-self-adjoint Schrödinger operators (the research direction proposed to him by his supervisor), had a strong influence on the field and attracted the attention of one of the most distinguished mathematicians of the 20th century, M.G. Krein, who wrote a letter expressing his appreciation of the outstanding work.

His second (Doctor of Sciences or Habilitation) thesis was devoted to a newly established field – the theory of self-adjoint dilations of dissipative operators and their applications in various problems of Mathematical Physics. Studies of these problems are connected with the names of B. Sz.-Nagy, C. Foias, R.S. Phillips and P.D. Lax, but Pavlov's extraordinary work made him one of the world's leading specialists in that specific field. A strong interest in applications was one of the main features of Pavlov's scientific activity. He liked to repeat the words said to him by R. Phillips: "Boris, keep close to applications". A combination of that interest with professional use of modern Complex Analysis and Operator Theory can be found in almost all of his papers, including the brilliant work on scattering theory on the Lobachevsky plane done in collaboration with L.D. Faddeev. That paper was the basis for the book *Scattering Theory for Automorphic Functions* by P.D. Lax and R.S. Phillips.

In addition, Boris Pavlov was a remarkable teacher and lecturer. People who attended his lectures forever remember his special style and his love for Mathematics which he tried to instill in his students. Unsurprisingly, he was the supervisor to an unusually large family of students (see below). His students will always remember the unusual care and understanding received from their mentor.

Concerning Pavlov's administrative activity, we mention that he was a Head of the Department of Higher Mathematics and Mathematical Physics (Faculty of Physics) and later of the Department of Mathematical Analysis (Faculty of Mathematics and Mechanics). He even worked as a vice-rector of Leningrad University. Here it is worth mentioning one fact which perfectly characterises his personality: when in 1981 he had to leave the vice-rector position — still being Head of the Dept. of Mathematical Analysis — he also resigned from the later position and returned to the Faculty of Physics as an ordinary professor. The reason was that Boris had earlier promised the Head of Mathematical Analysis position to Prof. S.A. Vinogradov and felt unable to allow himself to violated that promise, although at the time it was not so easy for him. In 1994, Pavlov moved to New Zealand, where he held a Personal Chair in Pure Mathematics at the University of

Auckland, later becoming a member of the Institute for Advanced Study at Massey University, Albany. He continued to work at the Saint Petersburg University as the Head of the Laboratory of Complex Systems Theory at the Physics Faculty.

Pavlov became a Fellow of the Royal Society of New Zealand in 2004 and a member of the Russian Academy of Natural Sciences in 2010.

Finally, just a few words about Pavlov's personality: he liked mountain skiing, kayak trips and many other activities typical for his generation. Moreover, he was a talented artist, and drawing was probably the second strongest passion in his life after Mathematics.

Pavel Kurasov
Ari Laptev
Sergey Naboko
Barry Simon

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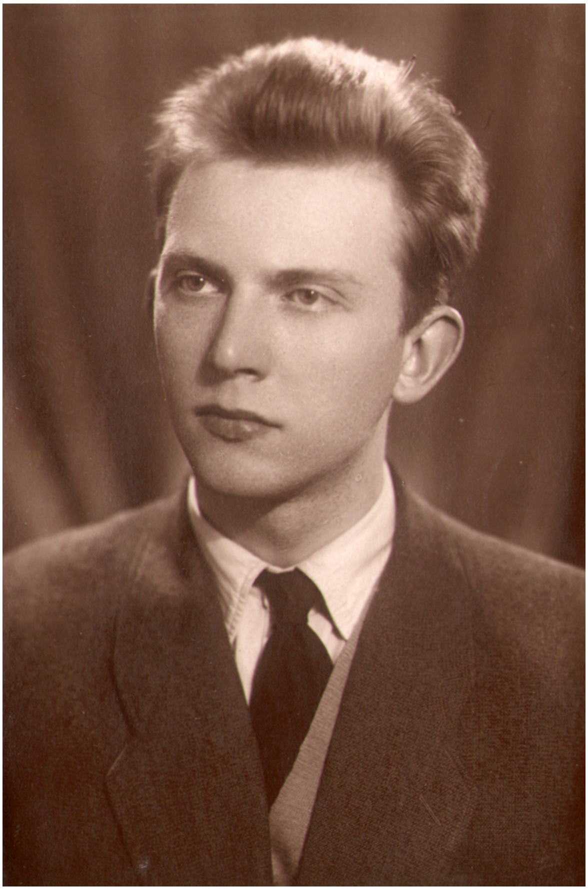
Part I

Boris Pavlov: Life and Mathematics



First year student, 1953

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Curriculum Vitae

Boris Pavlov
(Kronshtadt, Russia, 27 July 1936 – Auckland, New Zealand, 30 January 2016)

Educational Qualification
1959, Leningrad University, Faculty of Physics, grad. 1958.

Academic Degrees

1. Doctor of Sciences in Mathematical Analysis (Leningrad University, 1974), Title: "Dilation Theory and Spectral Analysis of Nonselfadjoint Differential Operators".
2. Ph.D. in Mathematical Analysis (Leningrad University, 1964), Title: "Spectral Investigation of Non-self-adjoint Operator $-y'' + qy$".

Positions Held

1. Professor (since Feb. 2009) in the Institute of Advanced Study at Massey University, Albany Campus, Auckland, New Zealand.
2. Head of the Laboratory (since Feb. 1995) of Quantum Networks at V. Fock Institute for Physics at the Faculty of Physics, Saint Petersburg University, Saint Petersburg, Russia.
3. Professor, Personal Chair in Pure Mathematics, Dept. of Mathematics, the University of Auckland, New Zealand, March 1994 – Dec. 2007. NZ-citizen since 2000.
4. Professor, Higher Mathematics and Mathematical Physics, Physics Faculty, Leningrad University [1982–1995].
5. Vice-rector of Leningrad University [1978–1981] (Research).
6. Chair of Analysis, Mech.– Mathem. Faculty, Leningrad University [1978–1982].
7. Professor, Higher Mathematics and Mathematical Physics, Physics Faculty, Leningrad University [1977–1978].
8. Associate Professor, Higher Mathematics and Mathematical Physics, Physics Faculty, Leningrad University [1966–1977].
9. Assistant professor, Department of Higher Mathematics and Mathematical Physics, Physics Faculty, Leningrad University [1961–1966].
10. Postgraduate student, Department of Higher Mathematics and Mathematical Physics, Physics Faculty, Leningrad University [1959–1961], supervisor Prof. M.S. Birman.

Significant Distinctions, Awards

- 1967 Distinguished Teaching Award of Leningrad University
- 1984 First Leningrad University Prize for Research
- 2004 Fellow of Royal Society of New Zealand
- 2010 Full member of Russian Academy of Natural Sciences.
- 2007 Silver Medal from the World exhibition of inventions, research and industrial innovation Brussels Eureka
  (with A. Pokrovski, E. Ryumtsev, T. Rudakova, A. Kovshik)
- 2007 Professor of category A (highest category in NZ scale awarded).

Professional Societies, Service, Other Activities

- Saint Petersburg Mathematical Society;
- New Zealand Mathematical Society;
- International association of Mathematical Physics.

Research Specialties, Career

Summary Statement

I am a specialist in Analysis and Mathematical Physics, a participant of Congresses of Mathematics in Poland 1983 and in Japan 1991, 1st Leningrad University prize for research (1984), Fellow of the Royal Society of New Zealand (2004), Full member or Russian Academy of Natural Sciences (2010).

Patents

1. Quantum Interference electronic Transistor (with G. Miroshnichenko) Patent 2062530, (Russia) Date of priority 12.03.1992.
2. Provisional Patent: A System and Method for Resonance manipulation of Quantum Currents Through Splitting Auckland University Limited, 504590, 17 May 2000, New Zealand.
3. Quantum Domain relay, United States Patent application 10/276,952, Patent Appl. Publication US 2003/0156781 A1, Aug. 21, 2003.

Research Interests

Spectral analysis of partial differential operators and Mathematical Physics. In particular: transport problems and scattering problems for Quantum Networks, fitted models of resonance scattering systems and analytic perturbation procedure.

List of PhD Students

1. **V.L. Oleinik** Master, PhD 1965–1971 (Docent, SPb Univ.)
2. **S.V. Petras** Master, PhD 1965–1970 (Docent, ITMO SPb)
3. **M.G. Suturin** Master PhD 1966–1971 (Docent, SPb Airspace Inst.)
4. **S.N. Naboko** Master, PhD 1969–1976 (Professor, SPb Univ.)
5. **S.A. Avdonin** Master, PhD 1969–1980 (Professor, Univ. Alaska Fairbanks)
6. **M.A. Shubova** Master, PhD 1969–1982 (Professor, Univ. New Hampshire)
7. **S.A. Ivanov** Master, PhD 1972–1978 (Researcher, SPb Inst. Control Proc.)
8. **I.Yu. Popov**, Master, PhD 1974–1979 (Professor, ITMO SPb)
9. **E. Il'in**, PhD 1984 (Leading researcher, Inst. for Regional Economics Studies of RAS, SPb)
10. **Yu.E. Karpeshina** Master, PhD 1975–1985 (Professor, Birmingham AL)
11. **K.A. Makarov** Master, PhD 1976–1982 (Professor, Univ. Missouri)
12. **S.E. Cheremshantsev** Master, PhD 1976–1982 (Professor, Orlean Univ.)
13. **A.V. Rybkin** Master, PhD student 1977–1982 (Professor, Univ. Alaska Fairbanks)
14. **A.V. Strepetov** Master, PhD 1978–1986 (SPb Airspace Inst.)
15. **M.D. Faddeev** PhD student 1982–1985 (Docent, SPb Univ.)
16. **P.B. Kurasov** Master, PhD 1981–1987 (Professor, Stockholm Univ.)
17. **V.V. Evstratov** Master, PhD 1984–1992 (now in business)
18. **A.A. Shushkov** PhD 1984–1987 (now in Canada)
19. **N.I. Gerasimenko** PhD 1985–1987 (Docent, Military Academy SPb)
20. **M.M. Pankratov** Master, PhD 1987–1991 (Insurance Comp., Sweden)
21. **S. V. Frolov** Master, PhD 1988–1993 (Professor, Techn. Refrig. Inst, SPb)
22. **A.A. Pokrovski** Master, PhD 1990–1995 (Researcher, SPb Univ.)
23. **R. Killip** Master, PhD (continued with B. Simon) 1994–1996 (Associate Professor, UCLA)
24. **M. Harmer** Master, PhD 1996–2000 (Lecturer, Otago Polytechnic)

Publications by Boris Pavlov

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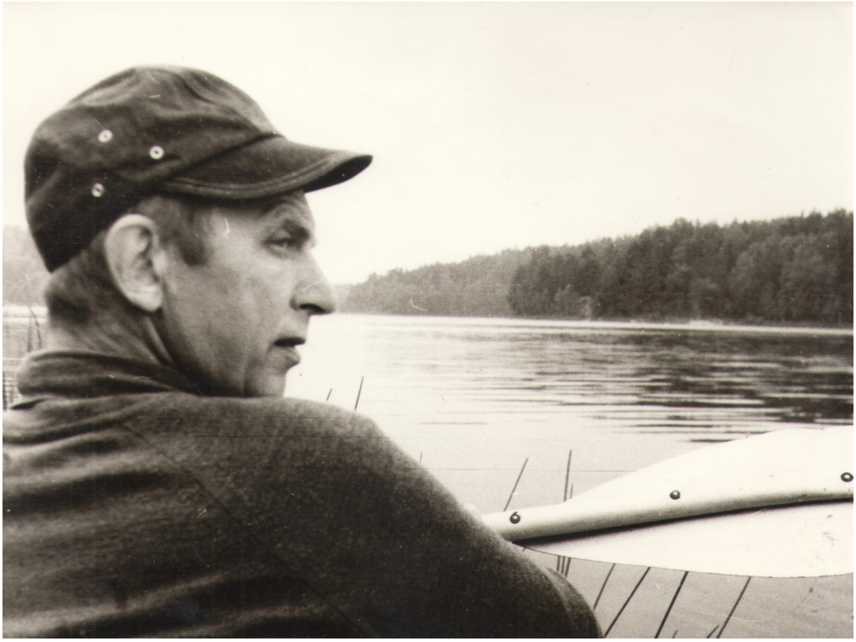
Photographs (private and academic life)

At Elbrus with wife Irina, 1966

In Latvia with daughter Anna, 1984
© I. Pavlova



Kayaking on Ladoga lake, 1985
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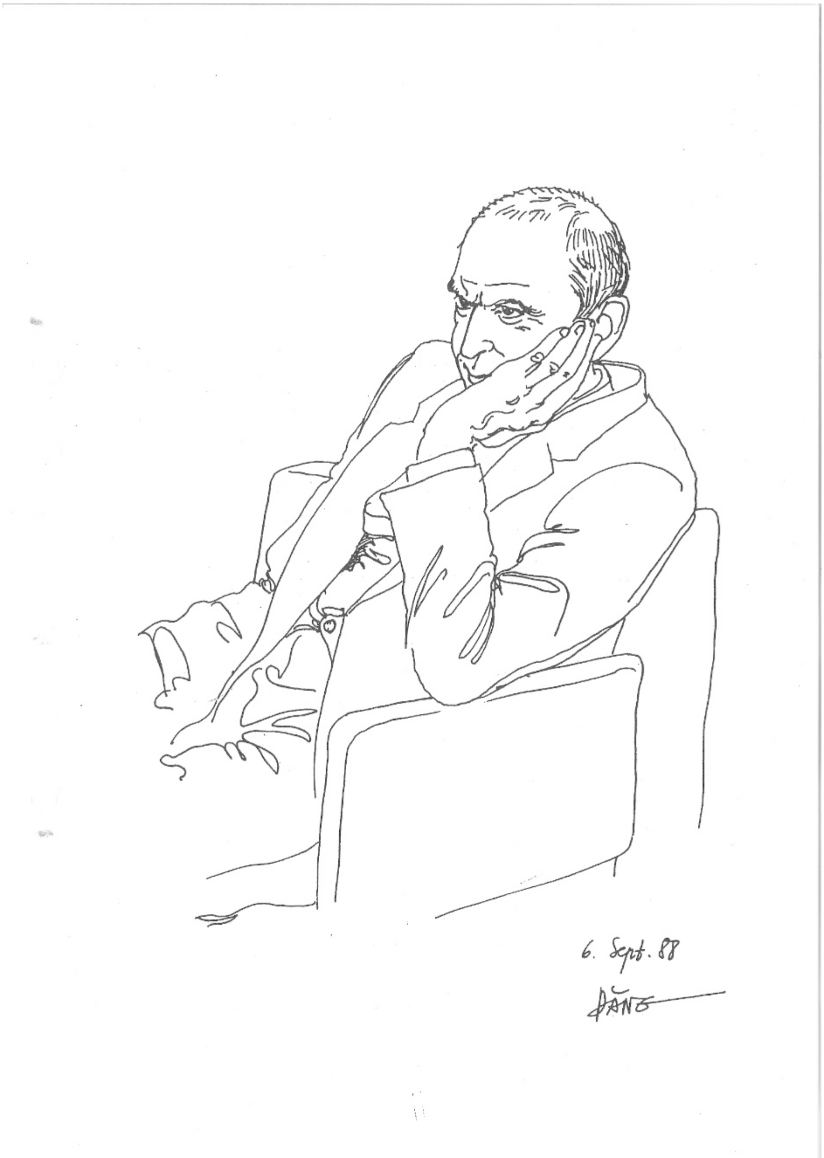

At a conference in Dubna, 1988

With P. Kurasov and S. Naboko in Gregynog, 2002
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Lecturing in Lund, 2006
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In Sweden, 2013
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With Pavel Kurasov and Jan Boman, 2013
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In Kronshtadt with daughter Anna, 2015
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With G.N. Fursey, 2015
receiving a diploma from the Russian Academy of Natural Sciences
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At summer house, 2015
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Boris Pavlov's attitude towards scientific research is perfectly reflected in Terenin's[1] rules, which Pavlov had displayed in his office in Leningrad and even took with him to New Zealand.

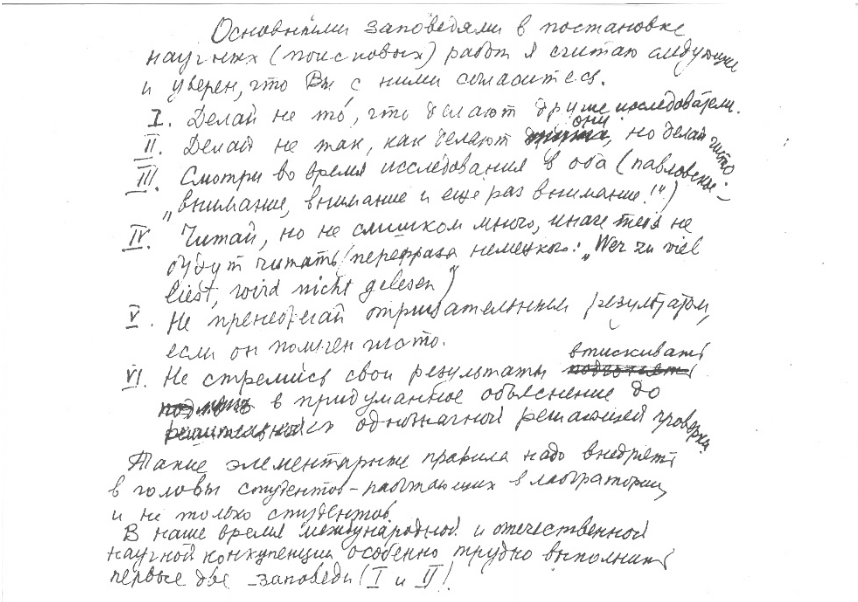
Academician A.N. Terenin's rules for researchers

I consider the following to be basic commandments in the formulation of scientific (research) works, and I am sure that you will agree with them:

- I Do not do what other researchers do.
- II Do not do it as they do; instead, do it cleanly.
- III When you research, look with both eyes (Ivan Pavlov's *Attention, attention and attention again*).
- IV Read, but not too much, otherwise your work will not be read (a rephrasing of the German: *Wer zu viel liest, wird nicht gelesen*).
- V Do not neglect a negative result if it was obtained correctly.
- VI Do not try to squeeze your results into invented explanations prior to an unequivocal crucial test.

Such elementary rules should be instilled into the minds of students working in laboratories, but not only students.

Nowadays, international and national scientific competition makes it particularly difficult to fulfil the first two commandments.


Основными заповедями в постановке научных (поисковых) работ я считаю следующие и уверен, что Вы с ними согласитесь.
I. Делай не то, что делают другие исследователи.
II. Делай не так, как делают они, но делай чисто.
III. Смотри во время исследования в оба (павловское: „внимание, внимание и еще раз внимание!")
IV. „Читай, но не слишком много, иначе тебя не будут читать (перефраза немецкого: „Wer zu viel liest, wird nicht gelesen")
V. Не пренебрегай отрицательным результатом, если он получен чисто.
VI. Не стремись свои результаты втискивать в придуманное объяснение до однозначной решающей проверки.
Такие элементарные правила надо внедрять в головы студентов-работающих в лабораториях и не только студентов.
В наше время международной и отечественной научной конкуренции особенно трудно выполнить первые две заповеди (I и II).

[1]Academician A.N. Terenin was a prominent physicist, one of the founders of photochemistry and photophysics research at Leningrad University.

Water-colours by Boris Pavlov

Suida river, 1975

Novgorod, 1970

Gatchina, park, 1980

Daughter Anna, 1980

Khibiny Mountains, 1985

Pavlov's Mathematics

P. Kurasov et al. (eds.), *Analysis as a Tool in Mathematical Physics*, Operator Theory: Advances and Applications 276, https://doi.org/10.1007/978-3-030-31531-3_2

Pavlov's contribution to science is not limited to his publications, he used to say that *papers should be written for political reasons.* Nevertheless, most of Pavlov's ideas are reflected in his publications showing us different facets of his scientific personality. A few years ago he summarised his achievements as follows:

My highest achievements are

1. Spectral theory of non-selfadjoint singular differential operators, 1962.
2. Riesz-basis property of exponentials on a finite interval, 1979.
3. Operator-theoretic interpretation of critical zeros of the Riemann zeta-function, 1972.
4. Symmetric Functional Model for dissipative operators, 1979.
5. Zero-range potentials with internal structure and solvable models, 1984.
6. Theory of the shift operator on a Riemann surface, jointly with S. Fedorov, 1987.
7. Modified analytic perturbation procedure ("Kick-start") for operators with eigenvalues embedded in the continuous spectrum, 2005.
8. Fitting of a zero-range solvable model of a quantum network based on rational approximation of the Dirichlet-to-Neumann map of the original Hamiltonian, 2007.
9. Fitting of a solvable model of stressed tectonic plates, in connection with prediction of powerful earthquakes, jointly with L. Petrova, 2008.
10. Quasi-relativistic dispersion and high mobility of electrons in Si–B sandwich structures, jointly with N. Bagraev, 2009.
11. Theoretical interpretation of the low-threshold field emission from carbon nano-clusters, jointly with Y. Fursey and A. Yafyasov, 2010.

One clearly sees that Pavlov ranked his fundamental contributions to pure analysis on the same level as his more recent work on applications, which stretched from dynamics of tectonic plates to semiconductors (see, for example, his posthumous paper with Victor Flambaum and Gaven Martin in the current volume).

The aim of this section is to describe Pavlov's research in pure analysis and operator theory, covering approximately the top half of the above list. Pavlov's work on non-self-adjoint operators (items 1 and 4) is well known to specialists as a base for modern theory of differential operators. The importance of the Pavlov–Faddeev paper (item 3) is best reflected by the book of P. D. Lax and R. S. Phillips, *Scattering Theory for Automorphic Functions*, for which the article served as *a starting point.* To complete the picture, we asked several world-leading experts, most of them long-time collaborators of Boris, to describe Pavlov's attitude towards analysis and mathematical physics, as well as his influence on the development of mathematics as a whole.

Zero-range potentials with internal structure and solvable models

V.M. Adamyan

The investigation of electron properties of polyatomic systems reduces, as a rule, to the spectral and scattering problems for the Schrödinger operator

$$H_V = -\frac{\hbar^2}{2m}\Delta + V(\mathbf{r})$$

in $\mathbb{L}_2(\mathbf{R}_3)$ with an effective self-consistent potential $V(\mathbf{r})$ that incorporates in some way the effect of electron–ion and electron–electron multi-particle interactions on a single valence electron. Less often under certain assumptions the description of electronic states of compounds is based on results of the spectral theory of self-adjoint operators in $\mathbb{L}_2(\mathbf{R}_3)$ formally given as the Laplace differential operator $-\Delta$ on a suitable set of functions $f(\mathbf{r})$ satisfying a variety of boundary conditions

$$\lim_{\rho_j \to 0}\left\{\frac{\partial}{\partial \rho_j}\rho_j f(\mathbf{r}) - b_j \rho_j f(\mathbf{r})\right\} = 0, \quad \rho_j = |\mathbf{r} - \mathbf{r}_j|, \tag{0.1}$$

for a given ensemble of points $\{\mathbf{r}_j\}$ and real numbers $\{b_j\}$. In applications to valence electrons of polyatomic systems $\{\mathbf{r}_j\}$ are positions of ions and $\{b_j\}$ are some parameters that account for the total influence of ions and other electrons on the single valence electron states. The latter approach is known as the the zero-range (or null-range) potential (ZRP) model. It is worth mentioning that the ZRP model can be applied and was applied more than once not only to the study of the electron structure and spectra of molecules and crystals. In fact, E. Fermi, who pioneered this model back in 1934, used it first to solve the problem of the shift of higher-order spectral lines in the presence of perturbing centers and then for the analysis of neutron scattering in substances that contain hydrogen. Examples of the use of ZRPs for modeling and simulation of real physical objects and phenomena can be found in the monograph [6].

The mathematical meaning of the ZRP model, which initially was associated with the formal differential operator

$$H = -\Delta + \sum_j b_j^{-1}\delta(\mathbf{r} - \mathbf{r}_j), \tag{0.2}$$

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was clarified by F.A. Berezin and L.D. Faddeev in the short note [5]. In fact, it was shown in [5] that instead of the incorrect expression (0.2) one should consider a certain self-adjoint extension of the symmetric Laplace operator $-\Delta_0$ defined on the set of smooth finite functions that vanish in a neighborhood of the given points, namely, the extension defined by the boundary conditions (0.1). This observation by F.A. Berezin and L.D. Faddeev became the starting point for numerous studies on the mathematical nature of ZRP models and their possible natural extensions and generalizations. The list of mathematical works directly related to this topic has long exceeded a thousand titles [4]. Among the works in this list, which contain fundamentally new approaches, objects and story lines related to the model being considered a prominent place is occupied by more than 50 articles and reviews authored or coauthored by B.S. Pavlov and numerous works of his disciples.

Returning to the ZRP model, we note that in the case of a single atom it gives poorer results than the potential model mentioned above. When it comes to reproducing the detailed structure and properties of real compounds, the approaches based on the ZRP model and those based on the potential model differ, loosely speaking, like a black-and-white drawing from an oil painting. However, for specific problems inherent to polyatomic systems, the ZRP model, remaining easily solvable, allows one to fully take into account the interference effects typical for multicenter systems, while the complexity of the potential model for such systems does increase.

An indisputable significant achievement of B.S. Pavlov is the far-reaching enrichment of the ZRP model by point potentials with internal structure. This greatly expanded the range of problems that can be treated by the generalized model and added colors to the black-and-white picture of its original version.

The special features of the ZRP model endowed with internal structure were first described by B.S. Pavlov and M.D. Faddeev in their short paper [8] without refering to ZRPs. To simulate one-electron states of a molecule interacting with its environment, the authors of [8] used a self-adjoint extension of the orthogonal sum of the above symmetric Laplace operator $-\Delta_0$ and (at first not associated with $-\Delta_0$) the closure L_0 of a symmetric Sturm–Liouville operator on a compact graph $\mathfrak{L}$ defined on the set infinitely differentiable functions that vanish near the vertices $\{\xi_j\}$ of the graph. In their analysis the vertices of the graph were identified with the assigned points $\{\mathbf{r}_j\}$ in the definition of $-\Delta_0$ and certain connecting self-adjoint boundary conditions were imposed at those points. The approach and constructions outlined in [8] with reference to a specific problem, gave impetus to numerous in-depth studies of B.S. Pavlov, his followers, and many other authors, devoted to deepening the ZRP method and developing a general theory of singular perturbations of self-adjoint operators.

The object studied in [8] was formalized in the subsequent paper [7], which apparently is the first place where the ZRP model with an internal structure was first explicitly described. Subsequently, B.S. Pavlov and under his obvious influence many other authors repeatedly turned to this richer model, refining it and finding significant applications of it in various problems of mathematical physics.

The first phase in the mathematical development of the ZRP model was originally based on the above-mentioned note [5] on von Neumann's theory of self-adjoint extensions of symmetric operators, and remained grounded on this theory right up to the publication of the papers [8, 7]. The results of these earlier investigations were summarized somewhat later in the monograph [3]. The more general model proposed in [7] did lead naturally to the theory of self-adjoint extensions with exit to a certain extended space containing a subspace associated with the internal states of point potentials. In the initial paper [8], a special self-adjoint extension A of the orthogonal sum of the operators $A_0 = -\Delta_0 \oplus L_0$ without exit from $\mathbb{L}_2(\mathbf{R}_3) \oplus \mathbb{L}_2(\mathfrak{L})$ for which the subspace $\{0\} \oplus \mathbb{L}_2(\mathfrak{L})$ remained invariant was compared from the viewpoint of scattering theory with an arbitrary self-adjoint extension A_1 of the same sum A_0 determined by suitable local boundary conditions at the points $\{\mathbf{r}_j \leftrightarrow \xi_j\}$. In the course of this study, a simple relationship was discovered between the analytic parameter in M.G. Kreĭn's formula for the resolvents of self-adjoint extensions A and A_1 of the operator A_0, on the one hand, and the scattering matrix for the pair A, A_1, on the other hand. In the general scattering problem for two self-adjoint extensions of the same symmetric operator with finite defect indices, the corresponding result was established in [1]. (The results and proofs of [1] remain valid also in the case of infinite defect spaces if for the pair of extensions in question the existence of wave operators is guaranteed.) As noted by B.S. Pavlov, the indicated relationship between M.G. Kreĭn's formula and the scattering matrix for a pair of extensions made it possible to understand the algebraic uniqueness of the ZRP models with internal structure, which ensures their solvability: the entire analysis reduces to the representation of the resolvent of the model Hamiltonian by Kreĭn's formula, after which it is already easy to investigate its spectral structure, calculate the scattering matrix, and often solve the inverse problem of reconstructing the interaction from spectral data.

In the process of solving the problems that emerged in [8] and also in the note [9], devoted to the construction of an explicitly solvable model of a small-opening resonator within the framework of extension theory, B.S. Pavlov undoubtedly gained insight into the essence of the ZRP model with internal structure and, more generally, into the so-called theory of singular perturbations, which, with respect to differential operators, reduces to perturbations of boundary conditions on manifolds of low dimension. This immediately sparked a rich research activity that revealed the features of natural generalizations and various applications of the ZRP model and the theory of singular perturbations. Thanks to the creative activity of students and close colleagues of B.S. Pavlov this research wave quickly spread throughout the world. In particular, numerous works by P. Kurasov and I. Popov made from the outset a substantial contribution in this direction (for an early bibliography, see [4]).

It should be recalled that numerous profound results on the spectral theory of dissipative operators were obtained by B. S. Pavlov with the ingenious use of the Lax–Phillips non-stationary approach to scattering theory. Beginning with the papers [8] and [9], B.S. Pavlov tried to use whenever possible this very effective (yet having a limited range of applications) approach to the scattering problems for Schrödinger and wave equations with ZRP potentials and singularly perturbed boundary conditions. He tried expand considerably the collection of exactly solvable physical problems by combining the ZRP model with internal structure, singular perturbations, and the Lax–Phillips approach. Unfortunately, he did not manage complete this task.

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Pavlov's perturbations

Sergey Khrushchev

Although I was not a direct student of Boris Sergeevich, he played a decisive role in my mathematical career. I got acquainted with him for the first time in our seminar on Complex Analysis in Leningrad. Occasionally, Boris Sergeevich visited it to report his results and also to formulate very interesting open questions. Just a few words to explain why Pavlov, being a member of a physics department, visited a mathematics seminar. Pavlov's first research was devoted to one-dimensional perturbations of self-adjoint operators which resulted in dissipative operators. To study them, Pavlov developed his own model, called now the symmetric model (I personally would suggest to call it Pavlov's model). By contrast, in those days our seminar was actually dealing with functional aspects of one-dimensional perturbations for unitary operators that result in contraction operators. The two subjects are related by well-known formulas. Questions considered in the seminar were mostly related to abstract mathematics, whereas in his talks, Pavlov showed us different problems, coming from physics. For this reason, Pavlov's talks usually made a great contribution to our seminar and led to progress.

One of Pavlov's problems was related to the description of continuous spectra of one-dimensional dissipative perturbations of Schrödinger operators with rapidly decreasing potentials. Pavlov showed that such spectra are sets of non-uniqueness for analytic functions in the upper half-plane with smooth boundary values in the Gevrey class $\mathbf{G}_\alpha$. Moreover, he showed that if such a set has Lebesgue measure zero and the intervals $\{l_\nu\}$ forming its complement satisfy the condition

$$\sum_\nu |l_\nu|^{\alpha \quad \varepsilon} < +\infty \tag{$*$}$$

for some $\varepsilon > 0$, then there is an outer function in $\mathbf{G}_\alpha$ with the set in question as its zero set. Such classes were considered previously by Lennart Carleson in his first paper in Acta Mathematica [1]. However, an intriguing question was to describe non-uniqueness sets for the class $\mathbf{G}_\alpha$. Stimulated by this important seminar talk of Pavlov, I started to think about this problem. It turned out to be quite difficult. The unusual feature of this problem, which distinguished it from similar problems considered by Carleson in [1], was that the answer could not be stated solely in

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terms of the lengths of the intervals forming the complement. The necessary and sufficient conditions I found (see [2]) were not simple, yet it still was possible to work with them. In particular, I showed that all previously known results follow from these conditions. Furthermore, I proved that for symmetric sets of Cantor type, condition $(*)$ is in fact necessary and sufficient. Also, there are pairs of sets with equal lengths of the intervals forming the complement, counting multiplicities, such that one of the sets is a set of uniqueness, while the other is not.

Soon after that Boris Sergeevich was appointed vice-rector of the Leningrad State University. He agreed with the rector that Friday would be his scientific day to communicate with his students. I still feel very proud for being included in this list of visitors. Later on, the Friday meetings turned into a course on inverse scattering problems. Pavlov delivered his lectures in Peterhof. This was one of the best Springs in my life. I left home and traveled by train to Peterhof. These were extraordinary lectures, both in the clarity of exposition and in the importance for applications. Later on, I used the lecture notes in the US to prepare a paper on continuous spectra of dissipative Schrödinger operators [3]. This course of Pavlov showed me how even such a difficult topic can be presented to students in a clear fashion. I still have at home in Saint Petersburg my hand-written lectures notes.

Once Boris Sergeevich visited our seminar shortly after my talk on an important paper of Muckenhoupt on the Riesz operators in weighted L^p spaces. What Pavlov presented on this occasion was very impressive, since he actually found necessary and sufficient conditions for a system of exponentials to form a basis in $L^2(-a, a)$. This work by Pavlov stimulated a series of papers, including my own paper [4] and our joint paper in Lecture Notes in Mathematics [5]. Some time later, I applied Pavlov's model and Bari's theorem to show that the abstract inverse scattering problem always has a solution, [6].

It was Pavlov who not only told me that I was ready for the defense of my doctoral thesis, but also helped to set up the whole process. Boris Sergeevich was a great diplomat. He didn't tell me details, but it turns out that he managed to convince L.D. Faddeev, who in those days decided everything in Mathematics in Leningrad , that I had enough material for the thesis. I think that otherwise I would have never been allowed to defend a doctoral thesis, regardless of what I could solve. The main problem with authoritative leaders is that they want to control everything but, in fact, can control only very few processes. This results in numerous mistakes and wrong decisions. Pavlov did personally face similar problems later. When he found a job in New Zealand and met Faddeev in Leningrad, Faddeev was angry because Pavlov did not ask his permission. Somehow Pavlov managed to fix the issue. However, later, when he returned to Saint Petersburg, he was not able to get any position in the Physics Department. He asked Faddeev for help, but the answer was negative, since Faddeev claimed that he could not do anything with people in the department.

My five-years fight with Faddeev for the Euler Institute, which he converted into a laboratory of Saint Petersburg division of the Steklov Institute so as to keep it under his control forever, clearly demonstrated that any question related to the personal needs of Faddeev could be solved. Just imagine: the conversion of the Euler Institute into a laboratory of a division of another institute was possible, but to create a position for Pavlov was impossible for him. Can you believe this? I cannot. This was just a classical example of a lie. If Faddeev insisted that Pavlov should ask his permission for a job in New Zealand, then why he could not solve Pavlov's problem when he returned? This rhetoric question has an obvious answer, but it looked as if nobody in the Saint Petersburg mathematical community cared. Thus Saint Petersburg University lost a great teacher. What was important was a unanimous support for any of Faddeev's wishes. So, what happened with Pavlov at the end of his life in Saint Petersburg was not at all a surprise for me.

The Doctor's diploma, which was awarded to me basically due to Boris Sergeevich's political efforts, helped me a lot in Almaty later on, allowing me a privileged access to the two main libraries in Kazakhstan. Using this access, I wrote what I think is the best mathematics paper in my life. This would have never happened should I have continued this long-term struggle.

At the beginning of my career in mathematics, I hesitated between the departments of physics and mathematics. Finally, I made my choice in favor of mathematics. Should I have chosen physics, I would have definitely been with Pavlov and his group. The result, I believe, would have been the same, except that my candidate thesis would not include the solution to the simultaneous approximation problem.

Pavlov had not only great talent, but also great intuition. Scientific interaction with him showed me that the intuition is the main driving tool in mathematical research. Before my contacts with Pavlov, I paid too much attention to Bourbaki. Now I think that no big theorem in Mathematics was proved Bourbaki's methods. Nevertheless, Bourbaki's approach in mathematics remains important for finding mistakes, or at least getting a feeling that something is wrong with some specific arguments.

Pavlov liked mountain skiing very much. Those times Boris Mityagin organized regular winter schools in Drogobyuch. There was a mountain resort nearby. So, once we both arrived to Drogobych with skis. Pavlov arranged a giant slalom track, and I followed him along many times. I thus managed to improve my skills considerably. His approach to mountain skiing was the same as to mathematics: one shouldn't try to demonstrate beautiful skiing, rather, one should aim for fast skiing. He told me that he called this"sculpting." Later, I rented with him a house in Kavgolovo for skiing.

With his death we all lost a great Man, a great Teacher, and a great Mathematician.

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Boris Pavlov and bases,
as I remember them

Nikolai Nikolski

Dedicated to the memory of Boris Pavlov,
a long-term friend and coauthor,
a remarkable mathematician with his fantastic ability
to foresee results before finding arguments,
and the only man I knew who could perceive mathematical theorems
as living physical systems.

Boris Pavlov, when I met him the first time, was a recent PhD student of Mikhail Birman at the Department of Physics of the LSU (Leningrad State University, now Saint-Petersburg State University). I suppose it happened around 1964–1965, when we both assisted on one of Birman's beautiful advanced courses in spectral theory of selfadjoint operators (delivered, due to a bureaucratic caprice, at the old building of the History Department of LSU, near the Twelve Colleges Building on Vasilievsky Island). Pavlov was already among the young prodigious celebrities of Saint Petersburg mathematical community, having discovered a complex spectral structure of extensions of symmetric differential operators (the so-called "nonphysical sheet" in scattering theory), mostly for Schrödinger operators.

This was exactly the field where B. Pavlov met the Riesz basis problem, especially for exponentials $e^{i\lambda_k x}$ as eigenfunctions of the operator $-y''$ with "spread" boundary conditions. Since the Riesz and unconditional basis problem was already among my own preoccupations, we rapidly found common interests and fields for a long lasting cooperation.

The Riesz and unconditional basis problem, especially for the exponentials, was for a long time among the pointed interests of analysts.

By definition (N. Bari (Bary) [8]), a *Riesz basis* (RB) (x_n) in a Hilbert space H is an isomorphic image ($x_n = Ve_n$) of an orthonormal basis (ONB) (e_n). An *unconditional basis* (UB) is a basis, i.e., every $x \in H$ can be uniquely represented in the form of a norm-convergent series

$$x = \sum_n a_n x_n$$

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($a_n \in \mathbb{C}$) and this series converges unconditionally, that is,

$$x = \lim_k S_{\sigma_k}, \ S_\sigma = S_\sigma(x) = \sum_{j\in\sigma} a_j x_j, \sigma \subset \mathbb{N},$$

for any sequence of finite subsets $\sigma_k \subset \mathbb{N}$, $\sigma_k \uparrow \mathbb{N}$.

In 1934, G. Köthe and O. Toeplitz have shown [20] that for *almost normalized* sequences (x_n) (i.e., such that $\|x_n\| \approx 1$, meaning that $0 < c \le \|x_n\| \le C < \infty$) in a Hilbert space, the property of being an unconditional basis is equivalent to the Riesz basis property (using Bari's language; the reason for the name "Riesz basis" was the Riesz–Fischer property of orthonormal bases that the coefficient space coincides with the space l^2, but "Fischer" disappeared at some point from the terminology...). E. Lorch [23] and M. Grinblyum [14] observed that (x_n) is an unconditional basis in H iff it is an isomorphic image ($x_n = Ve_n$) of an *orthogonal basis* (ON) (e_n). Some of these equivalences were independently found by R. Boas [10] and I.M. Gelfand [13].

One of the challenging problems of harmonic analysis and the theory of differential operators in the period 1930–1980 was to understand when a sequence of exponentials

$$\mathcal{E}_\Lambda = \left(e^{i\lambda_n t}\right)$$

is an unconditional basis in $L^2(I)$, I being an interval of $\mathbb{R}$. The studies for the case of infinite intervals started much later than those for finite intervals (although the latter case is more involved), but were completed first (see Sect. 2 below). The situation with finite intervals I turns out to be more delicate. Let us trace a few steps in the evolution of this subject.

1. First step – uniform proximity

The studies started with exponentials $x_n(t) = e^{i\lambda_n t}$ with real frequencies $(\lambda_n) \subset \mathbb{R}$ that are uniformly close to the harmonic ones $(n : n \in \mathbb{Z})$; by scaling and translating, we can always reduce the analysis to the setting of $L^2(I)$ with $I = (0, 2\pi)$. The spirit of this beginning stage was completely determined by the famous Paley–Wiener theorem [38] on "small perturbations" of the harmonic basis $(e^{int})_{n\in\mathbb{Z}}$ in $L^2(0, 2\pi)$:

Theorem. If $(\lambda_n)_{n\in\mathbb{Z}} \subset \mathbb{R}$ and $\delta := \sup_{n\in\mathbb{Z}} |n - \lambda_n| < 1/\pi^2$, then $\left(e^{i\lambda_n t}\right)$ is a Riesz basis in $L^2(0, 2\pi)$.

The proof is based on the observation that the linear operator $V : L^2 \to L^2$ acting as $Ve^{int} = e^{i\lambda_n t}$, $n \in \mathbb{Z}$, satisfies $\|I - V\| < 1$. Later on, R. Duffin and J. Eachus (1942) improved the computations, showing that $\delta < \log 2/\pi$ ($\sim 0.22\dots$) implies already the (RB) property for $(e^{i\lambda_n t})$, and finally M. Kadec [18] found the sharp sufficient condition $\delta < 1/4$ (for $\delta = 1/4$, counterexamples were known already to A. Ingham in the 1930s, see N. Levinson's book [22]).

2. Second step – generating and sine-type functions

In the next period, starting at the beginning of the 1960s, complex frequencies Λ were also allowed, and so were infinite intervals I. As a consequence of the Carleson interpolation theorem [12] and its basis interpretation in [42], the following theorem is stated in [37, 19] for the generic infinite interval $I = (0, \infty) = \mathbb{R}_+$:

Theorem. Let $\Lambda = \{\lambda_n\} \subset \mathbb{C}_+ = \{z \in \mathbb{C} : \operatorname{Im} z > 0\}$; then $\mathcal{E}_\Lambda$ is an unconditional basis in its (closed) span in $L^2(\mathbb{R}_+)$ if and only if Λ is a Carleson interpolating sequence for the half-plane $\mathbb{C}_+$ (written $\Lambda \in$ (C)).

Notice that $\mathcal{E}_\Lambda$ is never a basis (unconditional, or Schauder) in the whole space $L^2(I)$, with I an infinite interval. Interpolating sequences admit clear geometric descriptions, see, e.g., [32].

As to finite intervals I, $|I| < \infty$, the next step of the exponential basis problem was dominated by the use of the so-called "generating functions/sine-type functions". The research was limited to the question on *Riesz bases* $\mathcal{E}_\Lambda$, and so to frequencies Λ lying in a strip of finite width, parallel to the real axis. The idea of "generating function" can be traced back to [38], where it was used to treat the minimality and completeness properties of $\mathcal{E}_\Lambda$. But it was developed into a true theory only under the masterly hands of Boris Levin and his collaborators, see [21, 19] (and references therein). An entire function G_Λ of exponential type whose zero set coincides with Λ and for which the width of the indicator diagram is equal to the length of the interval I is called a *generating function* for the family $\mathcal{E}_\Lambda|I$. An entire function F of exponential type is called *a sine-type function* if its zero set is contained in a strip S of finite width, parallel to the real axis, and if $F|\partial S$ is an invertible function in $L^\infty(\partial S)$. The following results were obtained.

Theorem. (a) If Λ (lying in a strip) is separated, i.e.,

$$\inf_{n \neq k} |\lambda_n - \lambda_k| > 0$$

(a necessary condition), and if a generating function for $\mathcal{E}_\Lambda|I$ is a sine-type function, then $\mathcal{E}_\Lambda$ is a Riesz basis in $L^2(I)$ [21];

(b) If Λ satisfies the conditions of (a) above, and if (μ_n) is a separated sequence such that

$$|\operatorname{Re} \mu_n - \operatorname{Re} \lambda_n| \leq d \cdot \inf_{k, k \neq n} |\operatorname{Re} \lambda_n - \operatorname{Re} \lambda_k|$$

and $d < 1/4$, then $\mathcal{E}_M$ is a Riesz basis in $L^2(I)$, with $M = (\mu_n)$ [19].

In fact, S.A. Avdonin [1] found an even stronger sufficient condition for the (RB)-property of $\mathcal{E}_M$, replacing the uniform Kadets (Kadec)-type inequality in Katsnelson's theorem by a weaker condition of "closedness in the mean" of Λ and M. However, under certain restrictions on the frequency sets Λ and M, a kind of necessity of Katsnelson's proximity of a basis $\mathcal{E}_M$ to a "sine-type basis $\mathcal{E}_\Lambda$" was proved in [3].

Despite all these efforts and the beautiful theorems they produced, the adequate language for a solution of the Riesz basis problem was not yet found: neither the uniform proximity, nor sine-type functions could definitely settle the problem.

3. Third step – B. Pavlov's idea

Boris Pavlov's main idea appeared first in [39], and was subsequently developed in [40] into a complete theory that solved the *Riesz basis problem* for exponentials. The idea splits into the following two points:

(I) Consider the space $L^2(0,a)$, $a>0$, as a subspace of $L^2(\mathbb{R}_+)$ consisting of the functions f with $f(x)=0$ for $x>a$, and, assuming that $\Lambda\subset\mathbb{C}_+$, consider the exponentials on $(0,a)$ as orthogonal projections

$$P_a e^{i\lambda x}=e^{i\lambda x}\chi_{(0,a)}$$

of exponentials $\big(e^{i\lambda x}\big)_{\lambda\in\Lambda}$ in $L^2(\mathbb{R}_+)$ (notice that for a *Riesz basis of exponentials* $\big(e^{i\lambda x}\chi_{(0,a)}\big)_{\lambda\in\Lambda}$ in $L^2(0,a)$, the frequencies Λ lie always in a strip $\sup_{\lambda\in\Lambda}|\operatorname{Im}\lambda|<\infty$, and so the assumption $\Lambda\subset\mathbb{C}_+$ does not diminish generality, up to an isomorphic transformation $L^2(0,a)\to L^2(0,a)$, $f\mapsto e^{\alpha x}f$ with a large $\alpha>0$);

(II) Knowing already a Carleson-type criterion for Riesz basic sequences $\big(e^{i\lambda x}\big)_{\lambda\in\Lambda}$ in $L^2(\mathbb{R}_+)$ (see Sect. 2 above; for sequences in a strip, condition (C) coincides with the separation condition from Sect. 2 (a)), it remains to determine when the projection P_a is an isomorphism from

$$K:=\operatorname{span}_{L^2(\mathbb{R}_+)}\big\{e^{i\lambda x}:\lambda\in\Lambda\big\}$$

onto $L^2(0,a)$ (or "into", if looking for "Riesz basic sequences" $\big(e^{i\lambda x}\chi_{(0,a)}\big)_{\lambda\in\Lambda}$ in $L^2(0,a)$).

Using some known facts concerning the so-called Cartwright class of entire functions and defining a "canonical generating function" G (with $[-ia,0]$ as the growth diagram) by

$$G(w)=e^{iaw/2}\lim_{R\to\infty}\prod_{\lambda\in\Lambda,|\lambda|<R}\Big(1-\frac{w}{\lambda}\Big),$$

B. Pavlov showed that $P_a|K:K\to L^2(0,a)$ is a bounded invertible operator if and only if the operator $G\mathcal{H}G^{-1}$ is bounded, where $\mathcal{H}$ is the famous Hilbert transform

$$\mathcal{H}f(x)=\frac{1}{2\pi}\text{p.v.}\int_{\mathbb{R}}\frac{f(t)}{x-t}dt$$

(see Sect. 4 for more details). Finally, the main theorem of [40] is stated as follows.

Theorem. A family of exponentials $\big(e^{i\lambda x}\chi_{(0,a)}\big)_{\lambda\in\Lambda}$ is a Riesz basis in $L^2(0,a)$ if and only if

(a) $\sup_{\lambda\in\Lambda}|\operatorname{Im}\lambda|<\infty$,

(b) $\inf_{n\neq k}|\lambda_n-\lambda_k|>0$,
(c) $W := |G|^2$ satisfies the Hunt–Muckenhoupt–Wheeden condition (A_2) on a line $i\alpha+\mathbb{R}$, $\alpha\in\mathbb{R}$, parallel to the real line.

It is known that condition (A_2) can be replaced by the following equivalent *Helson–Szegö condition* (HS):

$$|G|^2 = e^{u+\tilde{v}},$$

where $u, v \in L^\infty(\mathbb{R})$ are real functions, $\tilde{v}$ stands for the harmonic conjugate, and $\|v\|_\infty < \pi/2$. Notice that the equivalence (HS) $\Longleftrightarrow$ (A_2) is known only because each of these conditions is equivalent to the boundedness of the Hilbert transform in the weighted space $L^2(\mathbb{R}, |G|^2dx)$; for details, see, for example, [34, Chap. 4]. It is interesting that B. Pavlov's paper [40] was printed in a row (in the same journal issue) with S. Hruschev's paper [16], which explained many important hidden nuances of the techniques and also showed how to derive all preceding results from Pavlov's results (condition (c) is always used in the (HS) form). Some other consequences of Pavlov's discovery are described in the next Sect. 4.

4. Post-Pavlov developments, unconditional bases

The first step after Pavlov's work was to overcome the framework of the Riesz bases and pass to general unconditional bases of exponentials (beyond the "almost normalization" condition), replacing condition (a) of Pavlov's theorem by the semi-boundedness condition $\inf_{\lambda\in\Lambda}\operatorname{Im}\lambda > -\infty$ (or symmetrically, $\sup_{\lambda\in\Lambda}\operatorname{Im}\lambda < \infty$). In fact, this trend started already in [40], where, however, the half-plane analog of condition (b) — the Carleson condition (C) — was imposed. This drawback was eliminated in [30] (and in the Russian "Nauka" 1980 edition of [32, pp. 256–257]:

Theorem. The Carleson condition (C) on the frequencies $i\alpha+\Lambda$, lying in the half-plane $\alpha+\inf_{\lambda\in\Lambda}\operatorname{Im}\lambda>0$, is necessary for the functions $\big(e^{i\lambda x}\chi_{(0,a)}\big)_{\lambda\in\Lambda}$ to form an unconditional basic sequence in $L^2(0,a)$.

Several other aspects distinguish the approach in [30] from the Pavlov–Hruschev approach: instead of exponentials, general *reproducing kernels* $\big(k_\zeta^\theta\big)_{\zeta\in Z}$ *of the model spaces* $K_\theta := H^2\ominus\theta H^2$ are considered, and the language of generating functions is replaced by that of the *Toeplitz operators* $T_{\theta\overline{B}}$ ($B = B_Z$ stands for the Blaschke product over Z (over Λ for exponentials)), which allowed to *separate the roles of* Λ *and* θ (the case of bases of exponentials corresponds to $\theta=\theta_a := e^{iax}$, $a>0$). Generally speaking, the usage of Toeplitz operators is based on Pavlov's ideas and the following identity, which holds for every pair of inner functions θ, Θ:

$$\theta J T_{\theta\overline{\Theta}} J\overline{\Theta} = \mathrm{id}_{H^2_-} \oplus (P_\theta \big| K_\Theta) \quad \text{on the space} \quad \Theta H^2_- = H^2_- \oplus K_\Theta,$$

where $Jf=\overline{zf}$ and P_θ stands for the orthogonal projection on K_θ (see [32, p. 334], or [31, p. 91]. This approach was then adopted in [17, 32, 33], as well as in a number of subsequent publications.

To be more specific, recall that it was clear for a long time that the problem of unconditional basic sequences of exponentials (i.e., bases in their *closed linear span*),

$$\left(e^{i\lambda x}\right)_{\lambda\in\Lambda} \quad \text{in } L^2(\mathbb{R}_+), \quad \Lambda\subset\mathbb{C}_+,$$

is equivalent (via the Fourier transform) to a similar problem for reproducing (Cauchy) kernels,

$$\left(\frac{1}{w-\overline{\lambda}}\right)_{\lambda\in\Lambda} \quad \text{in } H^2(\mathbb{C}_+) \quad \text{(the Hardy space)},$$

or (with a change of variables), to the analogous property of reproducing (Szegö) kernels in the unit disc $\mathbb{D}$,

$$\left(\frac{1}{1-\overline{\zeta}z}\right)_{\zeta\in Z} \quad \text{in } H^2(\mathbb{D}),\ Z\subset\mathbb{D}.$$

The case of the bases $(e^{i\lambda x})_{\lambda\in\Lambda}$ on a finite interval, say in $L^2(0,a)$, $\Lambda\subset\mathbb{C}_+$, corresponds to the case of reproducing kernel bases

$$\left(\frac{1-\theta(w)\overline{\theta(\lambda)}}{w-\overline{\lambda}}\right)_{\lambda\in\Lambda}$$

in a translation co-invariant subspace $K=H^2(\mathbb{C}_+)\ominus\theta H^2(\mathbb{C}_+)$, where $\theta=\theta_a:=e^{iaw}$.

Pavlov's solution to the Riesz bases problem for exponentials in $L^2(0,a)$ provided a sample recipe for settling the similar problem for general *"model spaces"* K_θ (θ stands for a (Beurling) inner function). Namely, in the unit disc setting and under the following "half-plane-type" frequency restriction

$$Z\subset\{\zeta:|\theta(\zeta)|\le q\}, \quad 0<q<1$$

(which coincides with $\inf_{\lambda\in\Lambda}\operatorname{Im}\lambda>0$ in the case of exponentials), the following criterion holds [30]:

Theorem. A family

$$K(Z,\theta):=\left(k_\zeta^\theta\right)_{\zeta\in Z}, \quad k_\zeta^\theta:=\frac{1-\theta(z)\overline{\theta(\zeta)}}{1-\overline{\zeta}z},$$

is an unconditional basis of the space $K_\theta=H^2(\mathbb{D})\ominus\theta H^2(\mathbb{D})$ if and only if $Z\in(\mathrm{C})$ and the Toeplitz operator $T_{\theta\overline{B}_Z}$ is invertible (i.e., if and only if $\theta\overline{B}_Z=c(\tilde{h}/h)$, where $|c|=1$ and h is an outer function satisfying (HS), and if and only if $\operatorname{dist}_{L^\infty}(\theta\overline{B}_Z,H^\infty)<1$ and $\operatorname{dist}_{L^\infty}(\overline{\theta}B_Z,H^\infty)<1$). (For the "unconditional basic sequence" property, the equivalent condition reduces to $Z\in(\mathrm{C})$ and $\operatorname{dist}_{L^\infty}(\theta\overline{B}_Z,H^\infty)<1$).

It is not completely clear what is the role of the above "half-plane-type" frequency restriction for the unconditional basis (UB) criteria. To be more specific, I *summarize below the known relationships* (see [17]) *between the four properties figuring in* (UB) *criteria:*

(I) $\sup_{\zeta\in Z}|\theta(\zeta)|<1$, (III) $T_{\theta\overline{B}_Z}$ *is invertible,*

(II) $Z\in(\mathrm{C})$, (IV) $\left(k_\zeta^\theta\right)_{\zeta\in Z}$ *is an (UB) in* K_θ,

as follows:

- (IV) $\Longrightarrow$ (II);
- (III) $\Longrightarrow$ (I);
- (II) & (III) $\Longrightarrow$ (IV) & (I),
- *but* (IV) $\not\Longrightarrow$ (I) (*and hence,* (IV) $\not\Longrightarrow$ (III))*; in particular, there are* UB*s with* $\lim_{\zeta\in Z}|\theta(\zeta)|=1$.

Modifying the language, one can obtain some other expressions for the (UB) property; for example, in [17, Sect. II.4] (and in [32, p. 210]), it is mentioned that property (II) (above) together with the invertibility of the operator $T: K_\theta\to K_B$, $f\mapsto P_BGf$, where G is a suitable H^2 function, is necessary and sufficient for the (UB) property (IV). The paper [11] developed another language that uses the Schur parameters for θ at points of Z, and furnished interesting new information on the geometry of reproducing kernels in K_θ.

The fact that *in the case of the exponentials*, the corresponding "half-plane" *condition* (I) ($\inf_{\lambda\in\Lambda}\operatorname{Im}\lambda>0$) can be omitted was shown in [27] (with a reasoning based on results obtained in [17]). This wrote the final chapter in the saga of exponential bases, as follows:

Theorem. If $\Lambda\subset\mathbb{C}$ and $\alpha\in\mathbb{R}$ is such that $(i\alpha+\Lambda)\cap\mathbb{R}=\emptyset$, then $(e^{i\lambda x})_{\lambda\in\Lambda}$ is an unconditional basis in $L^2(0,a)$ if and only if

(a) $\inf_{n\neq k}|\lambda_n-\lambda_k|>0$,
(b) $i\alpha+\Lambda_\pm\in(\mathrm{C})$ (for the corresponding half-plane),
(c) $W:=|G|^2$ satisfies the Hunt–Muckenhoupt–Wheeden condition (A_2) (on the line $i\alpha+\mathbb{R}$), where G stands for an appropriately defined generating function.

It is also known, see [28], that for frequencies Λ having a strip gap, $\Lambda\subset\{|\operatorname{Im}z|>d>0\}$, condition (c) above can be replaced by $\operatorname{dist}_{L^\infty}(\overline{\theta}_aB,H^\infty_\pm)<1$, where B is the Blaschke product for $\Lambda_+\cup\overline{\Lambda}_-$, $\Lambda_\pm=\Lambda\cap\mathbb{C}_\pm$. In an important paper [24], the authors introduce a large class of reproducing kernel L^p spaces of entire functions (the "weighted Paley–Wiener spaces") and provide (among other results) a complete characterisation of the reproducing kernel unconditional bases (in Pavlov's style: a generalized Carleson condition combined with an (A_p) condition for a kind of generating function).

5. Generalizations and applications

The applications of the above results have started even before the general theory flourished, specifically, for unconditionally convergent spectral decompositions of differential and integral operators, for "free interpolation" (in the Carleson–Shapiro–Shields style), for similarity problems in operator theory, for the control theory of systems "with distributed parameters". Later on, the reproducing kernels framework was developed (for model spaces, for de Branges, Fock, Dirichlet, and other spaces). It is impossible to give here a sufficiently representative survey of all these applications, generalizations, and links. Below, I restrict myself to a few thorough sources where the reader can find further references.

For earlier results/applications of B. Pavlov's work see [36, 37, 39], as well as the extensive survey of that time [35] (including bases of subspaces, multiple interpolation, etc., V. Vasyunin's basic results [43], and more).

For applications of the theory of unconditional bases (now classical) to the spectral theory of differential operators see [41, 15] (the latter (posthumous) book reprints all important papers of Gubreev and gives complete lists of references on the unconditional bases problem and its applications/relations to operator theory; in particular, Gubreev's more general point of view on bases of resolvent values $(\lambda I - A)^{-1}e, \lambda \in \Lambda$ of a given operator A is presented).

For various and important applications of exponential and reproducing kernel bases to control theory, see [2], [33, vol. 2], and references therein.

Generalizations and developments of the "theory of bases of reproducing kernels" as an independent subject were also numerous and important during last decades. The framework of this memorial essay does not allow me to quote and/or analyse them in any representative way. Instead, I am indicating below just a few recent results most closely related to Pavlov's operator approach. But first here is a list (in alphabetical order) of members of the community actively working in the field (restricted to exponentials and reproducing kernels): S. Avdonin, A. Baranov, Yu. Belov, A. Borichev, I. Boricheva, E. Fricain, P. Gorkin, G. Gubreev, A. Hartmann, K. Isaev, S. Ivanov, I. Joó, K. Kellay, A. Lunyov, Yu. Lyubarskii, N. Makarov, M. Malamud, A. Minkin, M. Mitkovski, B. Mityagin, A. Poltoratskii, K. Seip, B. Wick, D. Yakubovich, and R. Yulmukhametov.

Among the recent results on the topics discussed, I mention the following:

(1) A new important development of the "Toeplitz operator philosophy" in its applications to the geometry of exponentials is presented in the influential papers [25, 26]. In particular, for real-valued frequencies $\Lambda \subset \mathbb{R}$, the authors have modified the language, replacing $T_{\theta\overline{B}_Z}$ for $T_{\theta\overline{\Theta}}$, where Θ is for a meromorphic inner function having $\Theta(\lambda) = 1$, $\lambda \in \Lambda$; this opens the door to the world of de Branges spaces. For some specific classes of Λ's, further progress was made in [5] (not in the "Toeplitz language", but mostly in that of "de Branges spaces") and [29] (still using Toeplitz invertibility), leading to necessary and sufficient unconditional basis conditions for these Λ's.

(2) It was shown in [7] that (minimal) systems of reproducing kernels $\left(k_\zeta^\theta\right)_{\zeta\in Z}$ in K_θ are unitarily equivalent to systems of eigenvectors of rank-one perturbations of selfadjoint operators. (Earlier, such a statement was known only for perturbations having a *complete system of eigenvectors*.)

(3) A complete description of unconditional bases of the form $\left(k_\zeta^\theta\right)_{\zeta\in Z}$ was obtained for certain classes of inner functions θ (in particular, for Blaschke products with "lacunary" zeros), see [9, 6].
(4) Stability results for reproducing kernels unconditional bases (in the style of Kadec and Katsnelson) were obtained by E. Fricain and A. Baranov, see [4].

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The work of Pavlov on shift operators on a Riemann surface

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Prelude

Boris Pavlov's mathematical quest was centered on the interplay between operator theory, complex analysis, and mathematical physics. More specifically, he had an amazing vision relating the spectral analysis of an operator to nontrivial phenomena in function theory and to relevant properties of associated physical systems. The bilateral shift, its restriction the unilateral shift, compressions thereof to coinvariant subspaces, and vector-valued versions of all these, where of course central players in the story.

As far as I know, Boris was never particularly interested in multidimensional versions such as shifts in several complex variables. One reason may have been that he could not identify interesting physical models; indeed, these are still largely lacking, despite major progress of the last two decades in multivariable operator theory.

However, Boris became very interested in another generalization of the shift operator, from the unit disc to finitely connected domains (or more generally, finitely connected open Riemann surfaces), and made a major contribution to this fascinating topic in his joint work [39] with Sergei Fedorov. One motivation here is quite clear. If the discrete unitary evolution is constructed from a selfadjoint operator whose absolutely continuous spectrum consists of a single band $[a, b]$, the Lax–Phillips scattering scheme can be an effective tool for studying the (perturbed) dynamics using function theory on the simply connected domain $\mathbb{C} \setminus [a, b]$ via the conformal equivalence with the unit disc, see, e.g., [20] and the references therein. But there are natural situations when the absolutely continuous spectrum of the selfadjoint operator in question has a more complicated structure, e.g., it consists of several bands $[a_1, b_1], \ldots, [a_n, b_n]$. We then need, in the words of [20], to "develop a *modified* Lax–Phillips scattering theory based on the spectral theory of functions" on the multiply connected domain $(\mathbb{C} \cup \{\infty\}) \setminus \bigcup_{i=1}^{n} [a, b]$ (in the example discussed there, $n = 2$).

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Some background

The study of Hardy spaces and related topics in function theory on a multiply connected domain was of course not new (and the following references are by no means exhaustive). Parreau [38] and others defined Hardy spaces on multiply connected domains via harmonic majorants, and Ahlfors studied extremal problems for bounded analytic functions [3, 4]. In the process he established the fundamental fact that any finitely connected domain (in fact, any finitely connected open Riemann surface) can be represented as a finite branched covering of the unit disc (see [22] for a detailed survey on this topic). This was followed by the work of Widom [50, 51], who gave a precise characterization of the infinitely connected open Riemann surfaces that admit a sufficiently rich theory of Hardy spaces (they are usually referred to now as Riemann surfaces of Parreau–Widom type).

Meanwhile, an analogue of Beurling's representation for subspaces of the Hardy space on a finitely connected open Riemann surface S that are invariant under multiplication by bounded analytic functions on S have been obtained by Sarason [43] in the case of the annulus and by Forelli [21], Hasumi [24], and Voichick [47, 48] in the general case, while Voichick and Zalcman [49] established an analogue of the inner-outer factorization. These results were then generalized by Neville [36, 37] and Hasumi [25] to infinitely connected open Riemann surfaces of Parreau–Widom type. Finally, Abrahamse and Douglas [2] considered the case of vector-valued functions on a finitely connected domain, and Abrahamse [1] and Ball [9] studied interpolation problems.

One key and natural feature that distinguishes the multiply connected case is that even if one is interested in bona fide functions, it is necessary to consider multivalued functions that acquire multipliers of absolute value 1 when going around closed loops that generate the fundamental group. More precisely, these are character-automorphic (rather than automorphic) functions on the universal covering surface corresponding to a character of the fundamental group or equivalently, sections of a flat unitary line bundle. (In the vector-valued case, a character is replaced by a unitary representation of the fundamental group, and a flat unitary line bundle by a flat unitary vector bundle.)

Before discussing the paper of Pavlov–Fedorov [39] and its contributions, two comments are in order. The first one is on the level of methodology. Ahlfors' study of function theory on a finitely connected open Riemann surfaces S made an explicit use of the classical theory of compact Riemann surfaces via the so called (Schottky) double: this is a compact Riemann surface X that is obtained by taking a mirror image S' of S and gluing S and S' together along their common boundary; e.g., the double of an annulus is a torus. On the other hand, most of the work around the generalization of Beurling's theorem to the multiply connected setting used the lifting to the unit disc via the universal covering map $\mathbb{D} \to S$ (the first use of this in the Hardy space setting is probably due to Rudin [42]). While this provides a relatively quick way to some proofs, it usually lacks expliciteness.

The second comment is on a conceptual level. In function theory on the unit disc and related operator theory, Beurling's theorem is but the first step. Once one has a full description of invariant subspaces for the unilateral shift, one considers the restrictions of the adjoint operator, namely the backward shift, to its invariant subspaces, and develops a rich spectral analysis for these. These restrictions also turn out to be model operators for contraction operators of class C_{00} (i.e., such that T^n and T^{*n} both tend strongly to zero as $n \to \infty$).

A pair of contractive analytic functions that are unimodular on the boundary; the vector representation of Hardy and Lebesgue spaces

What is then the analogue in the multiply connected case? The answer of Pavlov and Fedorov is that *instead of considering a single operator of multiplication by z, we have to consider two operators of multiplication by Θ_0 and Θ_1* — two contractive analytic functions on S that are continuous and have absolute value 1 on the boundary. These functions can be then meromorphically continued to the second half S' of the double X of S, where they have poles at the mirror images of their zeroes on S. The two functions Θ_0 and Θ_1 have to be chosen so that together they separate (or at least generically separate) the points of S (equivalently, the pair (Θ_0, Θ_1) gives a birational embedding of the double X into the complex projective plane).

For the case of a doubly connected domain $S = (\mathbb{C} \cup \{\infty\}) \setminus ([-1, -a] \cup [a, 1])$ $(0 < a < 1)$ that is considered in [39], the authors construct the functions Θ_0 and Θ_1 explicitly by hand. They place themselves from the start in the setting of the double, i.e., the Riemann surface X of the algebraic curve $w^2 = (z^2 - a^2)(z^2 - 1)$. This is of crucial role in the follow-up papers of Fedorov [14, 15], which treat the case of higher connectivity through a systematic use of the theory of compact Riemann surfaces, much in the spirit of Ahlfors. It is also important since it allows the authors to use the orthogonal direct sum decomposition of the L^2 space of the boundary into the H^2 spaces on S and on S'. (To be precise, the authors consider the space $L^2(\partial S)$ with respect to a harmonic measure, and $H^2(S) \oplus H^2(S')$ has in fact codimension 1 in $L^2(\partial S)$, with the defect (the orthogonal complement) explicitly identified. There is a useful alternative technical way of considering L^2 spaces of half-order differentials rather than functions [26, 13, 7, 8] that avoids the need of choosing the harmonic measure and makes the defect subspace disappear.)

The unitary functions Θ_0 and Θ_1 allow Pavlov and Fedorov to build orthonormal bases in the spaces $H^2(S)$ and $L^2(\partial S)$ that are analogous to the basis of the powers of z in the case of the unit disc. Even more important, *it allows them to build an explicit isometric isomorphism* (the vector representation) *between these spaces and the corresponding $\mathbb{C}^2$-valued spaces on the unit disc.* This isomorphism is essentially induced by the two-sheeted branched covering $\Theta_0 \colon S \to \mathbb{D}$ (extending to $\Theta_0 \colon X \to \mathbb{C} \cup \{\infty\}$).

A different version of the vector representation appeared later in the work of Alpay and Vinnikov [7]. As it turns out, the vector representation intertwines the multiplication by Θ_0 with multiplication by z and multiplication by Θ_1 with multiplication by an explicit 2×2 rational matrix function, indicating a clear link with the later work of Agler and McCarthy [5].

The main results

With the vector representation at hand [39, Section 1], the authors turn to the study of subspaces of the Hardy space $H^2(S)$ that are invariant for the pair of commuting multiplication operators, namely the operators of multiplication by Θ_0 and Θ_1. Proceeding exactly along the same lines as in the case of the unit disc, they obtain [39, Section 3] an *explicit* Beurling-type representation. The representation of Pavlov and Fedorov is somewhat different than the description of Forelli, Hasumi, and Voichick, but the later can be recovered as a corollary. I want to emphasize once again that the authors construct the Beurling-type representation directly without lifting first to the universal covering. In essence, the universal covering has been replaced as the main technical tool by a finite branched covering of the domain onto the unit disc (and of its double onto the Riemann sphere).

Now that the cast of characters has been fully identified and the description of invariant subspaces $\mathcal{D}_+ \subseteq H^2(S)$ is available, the authors turn in [39, Chap. 4] to their main goal. They consider the restrictions of the adjoints of the multiplication operators by Θ_0 and Θ_1 to their invariant subpaces, namely the operators $P_{H^2(S)}\bar{\Theta}_0|_K$ and $P_{H^2(S)}\bar{\Theta}_1|_K$, where $K = H^2(S) \ominus \mathcal{D}_+$, or equivalently, the commutative semigroup of contractions with two generators, $P_{H^2(S)}\bar{\Theta}_0^{m_0}\bar{\Theta}_1^{m_1}|_K$, $m_0, m_1 \in \mathbb{Z}_+$. They develop a detailed spectral analysis for these operators along the same lines as in the classical case. Namely, they compute explicitly the resolvents and identify the spectra, which turn out to be given by the values of $\bar{\Theta}_0$ and $\bar{\Theta}_1$, respectively, on the subset $\sigma \subseteq S \cup \partial S$ consisting of the closure of zeroes and the support of the singular measure of the multivalued inner function B on S corresponding to the invariant subspace $\mathcal{D}_+$. They compute the (joint) eigenfunctions of the discrete spectrum, which are given by reproducing kernels for the Hardy space at the corresponding points, as well as the biorthogonal (joint) eigenfunctions of the adjoint operators $P_K\Theta_0|_K$ and $P_K\Theta_1|_K$. Much like in the case of the unit disc, the eigenfunctions form a complete system if and only if B has only simple zeroes and no singular inner factor. In this case the spectral expansions for the adjoint operators are interpolating series for these zeroes, and the authors show that these series converge (i.e., the eigenfunctions form a Riesz basis) if and only if the corresponding Carleson-type condition is satisfied.

Aftermath

Pavlov and Fedorov dealt in [39] only with the case of doubly connected domains. Fedorov generalized both the methods and the results to the case of arbitrary finitely connected domains in the complex plane in [14, 15], see also [16] (the treatment there can be adapted, with some modifications, to the case of arbitrary finitely connected open Riemann surfaces). The basic layout is similar, however many items that were immediate in the doubly connected case require now an extensive use of the classical theory of compact Riemann surfaces, in particular Abelian differentials and the Riemann–Roch theorem. This applies especially to the construction of a pair (or a triple) of contractive analytic functions that are unimodular on the boundary. The results of Fedorov here — which are, of course, motivated by the programme of Pavlov and Fedorov in [39]) — are a significant improvement over the results of Ahlfors in [3, 4]. They deserve to be better known, especially with the renewed interest in real fibered morphisms that are a higher dimensional generalization of finite branched coverings from finitely connected open Riemann surfaces onto the unit disc [27].

Fedorov's further work [17, 18, 19] deals with the angles between Hardy spaces of multivalued (character automorphic) functions on S and on S' with respect to a weighted L^2 product on the boundary ∂S (the analogues of the results of Helson and Szegö, Helson and Sarason, and Hunt, Muckenhoupt and Wheeden in the case of the unit disc) and the related estimates of projections from one coinvariant subspace onto another one. This is very much the next natural question in the programme laid out in [39]. It is remarkable that the author manages to obtain complete and explicit answers (which turn out to be character dependent). It would be interesting to apply the methods of these papers, which are a natural continuation of the methods of [39], to other problems in function theory on a multiply connected domain where no complete and explicit answers are known as yet. Interpolation problems, where the currently known citeria involve testing the positivity of a continuum of character-dependent Pick type matrices [1], could be a good candidate for such an application.

Some related developments

Spectral analysis in the Hardy space of the unit disc (or of the upper half-plane) is one of the two components of the usual theory of operator models. The other component is an identification of a large and natural class of abstract operators, namely contractions of class C_{00} (or dissipative operators such that e^{itT} tends strongly to zero as $t \to \infty$), that are (explicitly) unitarily equivalent to the restrictions of the (vector-valued) backward shift to its invariant subspaces.

The unilateral shift is the simplest instance of a subnormal operator. Abrahamse and Douglas [2], Xia [52, 53, 54], and Yakoubovich [55, 56, 57] have considered natural classes of subnormal operators which turn out to be unitarily equivalent to a multiplication operator in a Hardy space on a finitely connected domain or on a finitely connected open Riemann surface; see also the work of Putinar [40, 41] and Gustafsson and Putinar [23] on hyponormal operators with rank one self-commutator associated to a quadrature domain. However, all of these (with the exception of [12], see also [46], which continue the work of [55, 56]) do not consider the compressions of a shift operator on a multiply connected domain to its coinvariant subspaces.

In 1978, M.S. Livšic discovered [29, 30, 31] that a pair of commuting completely nonselfadjoint operators with finite non-Hermitian ranks satisfy a real polynomial equation in two variables. This was the starting point of an extensive theory of commuting nonselfadjoint or nonunitary operators (and associated overdetermined multidimensional systems) based on the theory of algebraic curves and compact Riemann surfaces [35, 45, 33, 10, 11]; see also [32, 34] for physical/biological models and [44, 6] for some recent developments. One of the central notions is that of a joint characteristic function (the analogue of the characteristic function in the usual operator model theory) which is a mapping of vector bundles over a compact real Riemann surface. While there is some overlap with the tools developed by Pavlov and Fedorov in [39] and their generalizations, this theory is largely complementary. Much like the work of Livšic and his collaborators and of Sz.-Nagy and Foias in the single operator case, it provides explicit functional models for commuting dissipative operators with finite non-Hermitrian rank or commuting contractions with finite defects in coinvariant subspaces in Hardy spaces on a finitely connected open Riemann surface. It would be interesting to apply Pavlov's spectral analysis in these Hardy spaces to obtain further and finer results in the spectral theory of commuting nonselfadjoint and nonunitary operators.

Epilogue

Although Pavlov had several clear ideas that he shared, he never had the time or the opportunity to investigate in detail physical models where a Lax–Phillips type scattering theory would be naturally related to spectral analysis in the Hardy space on a multiply connected domain. The paper [20, Sect. 6], which is based on the work of Kurasov [28], presents a concrete example that still awaits being worked out, very likely showing a path for new developments.

The verses of Tyutchev that we never know how our words will resonate apply to natural philosophers as well as to poets.

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Part II

Research Papers

Singular perturbations of unbounded selfadjoint operators. Reverse approach

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In memory of Boris Pavlov: brilliant mathematician and fascinating personality

Abstract. Let A and A_1 be unbounded selfadjoint operators in a Hilbert space $\mathcal{H}$. Following [3], we call A_1 a *singular* perturbation of A if A and A_1 have different domains $\mathcal{D}(A), \mathcal{D}(A_1)$ but $\mathcal{D}(A) \cap \mathcal{D}(A_1)$ is dense in $\mathcal{H}$ and $A = A_1$ on $\mathcal{D}(A) \cap \mathcal{D}(A_1)$. In this note we specify without recourse to the theory of selfadjoint extensions of symmetric operators the conditions under which a given bounded holomorphic operator function in the open upper and lower half-planes is the resolvent of a singular perturbation A_1 of a given selfadjoint operator A.

For the special case when A is the standardly defined selfadjoint Laplace operator in $\mathbf{L}_2(\mathbb{R}^3)$ we describe using the M.G. Krein resolvent formula a class of singular perturbations A_1, which are defined by special selfadjoint boundary conditions on a finite or spaced apart by bounded from below distances infinite set of points in $\mathbb{R}^3$ and also on a bounded segment of straight line embedded into $\mathbb{R}^3$ by connecting parameters in the boundary conditions for A_1 and the independent on A matrix or operator parameter in the Krein formula for the pair A, A_1.

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1. Introduction

The so called solvable models associated with zero-radius potentials [2] and more general singular perturbations has come to the foreground in the late oeuvre of

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Boris Pavlov. He and his numerous disciples and followers enriched these models and significantly expanded the boundaries of their applications, endowing the involved point potentials and singular perturbations with internal structures. The results pertaining to the initial stages of the relevant studies can be found in the review [8] and subsequent monograph [3]. Recall that Schrödinger operators with zero-range potentials appeared in physical applications more than 80 years ago (historical references and comments can be found in the well-known books [5, 2, 3]). However, a clear understanding of the mathematical nature of these objects was achieved much later in [4]. After the note [4] the theory of extensions of symmetric operators turned out the main tool for solving the problems of spectral theory and scattering theory for Schrödinger and afterwards for Dirac operators with potentials or analogues of potentials formally given as combinations of Dirac δ-functions.

As it was traced in [1, 8], the solvability of the zero-range potential models and problems for a wide class of singular perturbations of selfadjoint operators lie in the algebraic simplicity and universality of M.G. Krein resolvent formula for selfadjoint perturbations of a given selfadjoint operator. It appears that to solve specific problems of spectral and scattering theory for sufficiently wide class of perturbations of selfadjoint operators the mentioned M.G. Krein formula can be used as the only tool of analysis.

However, despite the large number of deep and interesting mathematical results on the zero-range potential models and singular perturbations and their effective, elegant and useful physical applications obtained in subsequent years, a profound analysis of related problems with quest for analytically solvable models does not apply to interests of the majority of today's consumers of mathematical physics. Instead, they would prefer to solve their problems using computer algebra systems and numerical calculations. This paper is an attempt to develop an available to the mass consumer simplified theory of singular perturbations of seladjoint operators dealing only with that resolvent formula.

In auxiliary Sect. 2, we recall the necessary and sufficient conditions under which a function on an open set of the complex plane whose values are bounded linear operators in Hilbert space is a resolvent of densely defined closed linear operator, particularly, of selfadjoint operator. We also give here the known description of resolvents for finite-dimensional selfadjoint perturbations of a given selfadjoint operator.

A short Sect. 3 is devoted to the derivation of the Krein formula for resolvents of certain classes of singular perturbations of a given selfadjoint operator. Using the approach of M.G. Krein, but not referring to the theory of extensions, we justify a well-known, in our opinion application-friendly parametrizations of this formula.

The first of two obtained versions of the Krein formula is illustrated in Sect. 4 by the example of singular selfadjoint perturbations of the selfadjoint Laplace operator in $\mathbf{L}_2(\mathbb{R}^3)$ that have form of a sum of zero-range potentials spaced apart by bounded from below distances.

The second obtained version of the Krein formula is more suitable for describing singular perturbations of the classical Laplace operator in $\mathbf{L}_2(\mathbb{R}^3)$ whose action is concentrated on one- and two-dimensional manifolds in $\mathbb{R}^3$. This version was illustrated in Sect. 5 by singular perturbation of the Laplace operator, which is located on a straight-line segment embedded into $\mathbb{R}^3$. The role of the parameter in the Krein formula in this case is played by the selfadjoint Sturm–Liouville operator on the given segment. The results of this section can easily be extended to the case when the singular perturbation of the Laplace operator in $\mathbf{L}_2(\mathbb{R}^3)$ is given on a compact quantum graph embedded into $\mathbb{R}^3$. In the latter case, we obtain an extension of the proposed in [9] model for describing the interaction of molecules with the surrounding medium.

2. Reminder of resolvents' basic properties

Theorem 2.1. *Let $R(z)$ be a strongly continuous operator function on a nonempty open domain $\mathbb{D}$ of complex plane and values of this function are bounded operators in a Hilbert space $\mathcal{H}$. $R(z)$ is the resolvent of a linear densely defined closed operator A in $\mathcal{H}$ with the resolvent set $\varrho(A) \supseteq \mathbb{D}$ if and only if*

- $$\ker R(z) = \ker R(z)^* = \{0\}; \tag{2.1}$$
- *$R(z)$ is holomorphic on $\mathbb{D}$ and for any $z_1, z_2 \in \mathbb{D}$ the Hilbert identity*
$$R(z_1) - R(z_2) = (z_1 - z_2)R(z_1)R(z_2) \tag{2.2}$$
hold.

Proof. By (2.1) for each $z \in \mathbb{D}$ the linear relation

$$\begin{cases} g = R(z)f, \quad f \in \mathcal{H}, \\ A_z g = f + zR(z)f = f + zg \end{cases} \tag{2.3}$$

defines a linear operator A_z with the dense domain $R(z)\mathcal{H}$ and such that the range of $A_z - zI$ is $\mathcal{H}$.

If for some sequence $f_n \in \mathcal{H}$ the sequences $g_n = R(z)f_n$ and $A_z g_n = f_n + zg_n$ converge to vectors g_∞ and h_∞, respectively, then by virtue of (2.3) the sequence f_n converges to some vector f_∞. Since $R(z)$ is a bounded operator, then $g_\infty = R(z)f_\infty$. Therefore and g_∞ belongs to the domain of A_z and

$$A_z g_\infty = f_\infty + zg_\infty = \lim_{n\to\infty} (f_n + zg_n) = \lim_{n\to\infty} A_z g_n = h_\infty,$$

that is A_z is a closed operator.

According to (2.2), for any $z_1, z_2 \in \mathbb{D}$ we have $R(z_1)R(z_2) = R(z_2)R(z_1)$ and

$$R(z_2)\mathcal{H} = R(z_1)[I + (z_2 - z_1)R(z_2)]\mathcal{H} \subseteq R(z_1)\mathcal{H}.$$

Hence the domains of all A_z coincide.

Taking some $g = R(z_1)f = R(z_2)[I + (z_1 - z_2)R(z_1)]f,\ f \in \mathcal{H}$, we obtain with account of (2.3), (2.2) that

$$\begin{aligned} A_{z_2}g &= [I + (z_1 - z_2)R(z_1)]\, f + z_2R(z_2)\, [I + (z_1 - z_2)R(z_1)]\, f \\ &= A_{z_1}g + z_2\, \{-R(z_1)f + R(z_2)f + (z_1 - z_2)R(z_1)R(z_2)f\} = A_{z_1}g. \end{aligned}$$

Therefore the action of A_z does not depend on z and for the operator $A \equiv A_z,\ z \in \mathbb{D}$, by construction

$$(A - zI)^{-1} = (A_z - zI)^{-1} = R(z), \tag{2.4}$$

which is the desired conclusion.

The proof of "only if" part is trivial. □

Theorem 2.2. *If $R(z)$ as in Theorem 2.1 and in addition*

$$z \in \mathbb{D} \Longleftrightarrow \bar{z} \in \mathbb{D}, \tag{2.5}$$

$$R(\bar{z}) = R(z)^*, \quad z \in \mathbb{D}, \tag{2.6}$$

then $R(z)$ is the resolvent of a selfadjoint operator A.

Proof. As mentioned in the proof of Theorem 2.1, the range of $A - zI$ for $A = A_z,\ z \in \mathbb{D}$, defined by linear relation (2.3) is the whole space $\mathcal{H}$. Therefore it suffices to show that A is a symmetric operator. But for any $g_1 = R(z)f_1,\ g_2 = R(z)f_2,\ f_1, f_2 \in \mathcal{H},\ z \in \mathbb{D}$, by virtue of (2.6) and (2.2),

$$\begin{aligned} (Ag_1, g_2) - (g_1, Ag_2) &= ([f_1 + zR(z)f_1], R(z)f_2) - (R(z)f_1, [f_2 + zR(z)f_2]) \\ &= ([R(\bar{z}) + zR(\bar{z})R(z) - R(z) - \bar{z}R(\bar{z})R(z)]f_1, f_2) = 0. \end{aligned}$$ □

Theorem 2.3. *Let A be a selfadjoint operator in $\mathcal{H}$; $R(z)$,* $\mathrm{Im} z \neq 0$, *is the resolvent of A; $f_1, \ldots, f_N$, $1 \leq N \leq \infty$, are linearly independent vectors from $\mathcal{H}$; $Q(z)$ is the Nevanlinna $N \times N$-matrix function with the elements*

$$q_{mn}(z) = (R(z)f_n, f_m)\,, \quad 1 \leq m, n \leq N. \tag{2.7}$$

Then for any invertible Hermitian $N \times N$ matrix $W = (w_{mn})_1^N$ the matrix $Q(z) + W$, $\mathrm{Im} z \neq 0$, *is invertible and the operator function*

$$R_1(z) = R(z) - \sum_{m,n=1}^{N} \left([Q(z) + W]^{-1}\right)_{mn} (\cdot, R(\bar{z})f_n)\, R(z)f_m \tag{2.8}$$

is the resolvent of a selfadjoint operator A_1.

Proof. By our assumptions $Q(z)$ (as well as $Q(z) + W$) is a Nevanlinna matrix function with the imaginary part

$$\frac{1}{2i}\, [Q(z) - Q(z)^*]$$

having property

$$\begin{aligned} \frac{1}{z - \bar{z}}\, [Q(z) - Q(z)^*] &= ((R(z)f_m, R(z)f_n))_{m,n=1}^N \\ &= \Gamma(R(z)f_1, \ldots, R(z)f_N) \geq \lambda_{\min}(R(z)f_1, \ldots, R(z)f_N)I, \end{aligned}$$

where $\Gamma(R(z)f_1,\dots,R(z)f_N)$ is the Gram–Schmidt matrix for vectors

$$R(z)f_1,\dots,R(z)f_N$$

and $\lambda_{\min}(R(z)f_1,\dots,R(z)f_N)$ is the minimal eigenvalue of $\Gamma(R(z)f_1,\dots,R(z)f_N)$. Since vectors $f_1,\dots,f_N$ are linearly independent and $\ker R(z)=\{0\}$,

$$\lambda_{\min}(R(z)f_1,\dots,R(z)f_N)>0.$$

Hence $Q(z)+W$ is invertible.

Suppose that $R_1(z)h=0$, $\mathrm{Im} z\neq 0$ for some $h\in\mathcal{H}$, that is,

$$R(z)h=\sum_{m,n=1}^{N}\left([Q(z)+W]^{-1}\right)_{mn}(h,R(\bar z)f_n)\,R(z)f_m. \tag{2.9}$$

Hence $R(z)h$ is a linear combination of the vectors $R(z)f_1,\dots,R(z)f_N$ and in view of invertibility of $R(z)$ we see that $h=\alpha_1 f_1+\cdots+\alpha_N f_N$ with some coefficients $\alpha_1,\dots,\alpha_N$. By (2.8),

$$R_1(z)f_j=\sum_{m=1}^{N}\left([Q(z)+W]^{-1}W\right)_{mj}R(z)f_m,\quad j=1,\dots,N.$$

Therefore

$$\begin{aligned}0&=R_1(z)h=R(z)\left(\beta_1 f_1+\cdots+\beta_N f_N\right),\\ \beta_m&=\sum_{m=1}^{N}\left([Q(z)+W]^{-1}W\right)_{mj}\alpha_j.\end{aligned} \tag{2.10}$$

Since $\ker R(z)=\{0\}$ and $f_1,\dots,f_N$ are linearly independent, $\beta_1=\cdots=\beta_N=0$. But if W is invertible then, by virtue of invertibility of $Q(z)+W$ and (2.10), $\alpha_1=\cdots=\alpha_N=0$, that is, $h=0$. Hence $\ker R_1(z)=0$.

Relation $R_1(z)^*=R_1(\bar z)$ follows directly from (2.8) because

$$R(z)^*=R(\bar z),\quad Q(z)^*=Q(\bar z),\quad W^*=W.$$

Taking into account that for $R(z)$ the Hilbert identity holds and that for $1\le m,n\le N$ and $\mathrm{Im} z_1,z_2\neq 0$,

$$\begin{aligned}q_{mn}(z_2)-q_{mn}(z_1)&=[q_{mn}(z_2)+w_{mn}]-[q_{mn}(z_1)+w_{mn}]\\ &=(z_2-z_1)\left(R(z_1)f_n,R(\bar z_2)f_m\right),\end{aligned}$$

one can easily verify by elementary algebraic manipulations that for $R_1(z)$ the Hilbert identity also holds.

We see that $R_1(z)$ satisfies all conditions of Theorems 2.1 and 2.2, which implies the desired conclusion. □

Remark 2.4. Comparing the formal inverse for operators in the left- and right-hand sides of (2.8) yields

$$A_1=A+\sum_{m,n=1}^{N}\left(W^{-1}\right)_{mn}(\cdot,f_n)\,f_m\,, \tag{2.11}$$

that is, if $N < \infty$, then A_1 is a finite-dimensional perturbation of A.

Remark 2.5. Let W in (2.8) be not invertible and

$$\mathcal{A} = \left\{h \in \mathcal{H} : h = \alpha_1 f_1 + \cdots + \alpha_N f_N,\ (\alpha_1, \ldots, \alpha_N)^T \in \ker W\right\}.$$

Then $R_1(z)h \equiv 0$ for any $h \in \mathcal{A}$ but in this case the restriction to $R_1(z)$ on the subspace $\mathcal{A}^\perp = \mathcal{H} \ominus \mathcal{A}$ is the resolvent of selfadjoint operator A_1 in $\mathcal{A}^\perp$.

Indeed, in the course of proof of Theorem 2.1 it was actually shown that $\ker R_1(z) = \mathcal{A}$. Since $R_1(z)^* = R_1(\bar{z})$, then $R_1(z)\mathcal{A}^\perp \subseteq \mathcal{A}^\perp$ and for the restriction of $R_1(z)$ to the invariant subspace $\mathcal{A}^\perp$ all conditions of Theorems 2.1 and 2.2 hold.

Specifically, if $W = 0$ in (2.8) and A is a bounded operator, then $P_{\mathcal{A}^\perp} R_1(z)|_{\mathcal{A}^\perp}$ where $P_{\mathcal{A}^\perp}$ is the orthogonal projector on $\mathcal{A}^\perp$ is the resolvent of selfadjoint operator $P_{\mathcal{A}^\perp} A|_{\mathcal{A}^\perp}$ in $\mathcal{A}^\perp$.

3. M.G. Krein's line of argument

M.G. Krein was the first who realized that the statement of Theorem 2.3 can be strengthened in the following way.

Theorem 3.1. *Let A be an unbounded selfadjoint operator in $\mathcal{H}$ and $R(z)$, $\operatorname{Im} z \neq 0$, is the resolvent of A; $\{g_n(z)\}_{n=1}^N$, $1 \le N \le \infty$, is the set of $\mathcal{H}$-valued holomorphic in the open upper and lower half-planes vector functions satisfying the conditions*

- *for any non-real z, z_0*

$$g_n(z) = g_n(z_0) + (z - z_0)R(z)g_n(z_0), \quad j = 1, \ldots, N; \tag{3.1}$$

- *at least for one non-real z_0 vectors $\{g_n(z_0)\}_{n=1}^N$ form a basis (Riesz basis if $N = \infty$) in their (closed if $N = \infty$) linear span $\mathcal{N}$ and none of non-zero vectors from $\mathcal{N}$ belong to the domain $\mathcal{D}(A)$ of A;*

$Q(z)$ is a holomorphic in the open upper and lower half-planes $N \times N$-matrix function (that generates a bounded operator in the space $\mathfrak{l}_2$ if $N = \infty$) such that

- *$Q(z)^* = Q(\bar{z}),\ z \neq 0$;*
- *for any non-real z, z_0*

$$Q(z) - Q(z_0) = (z - z_0)\left((g_m(z), g_n(\bar{z}_0))\right)_{1 \le m,n \le N}^T. \tag{3.2}$$

Then for any Hermitian $N \times N$ matrix $W = (w_{mn})_1^N$ (such that the closure of the linear operators defined as multiplication by W on a set of $\mathfrak{l}_2$-vectors with a finite number of non-zero coordinates is a selfadjoint operator in $\mathfrak{l}_2$ if $N = \infty$) the matrix (operator in $\mathfrak{l}_2$ if $N = \infty$) $Q(z) + W$, $\operatorname{Im} z \neq 0$, is (boundedly) invertible and the operator function

$$R_1(z) = R(z) - \sum_{m,n=1}^{N} \left([Q(z) + W]^{-1}\right)_{mn} (\cdot, g_n(\bar{z}))\, g_m(z) \tag{3.3}$$

is the resolvent of some selfadjoint operator A_1.

Proof. If $\{g_n(z_0)\}_{n=1}^N$ is a (Riesz) basis in $\mathcal{N}$ for some non-real z_0, then $\{g_n(z)\}_{n=1}^N$ is a (Riesz) basis in $\mathcal{N}$ for any non-real z. Indeed, by (3.1)

$$g_n(z) = U_{z_0}(z) g_n(z_0), \quad U_{z_0}(z) = (A - z_0 I) \cdot (A - zI)^{-1}, \tag{3.4}$$

and for any non-real z, z_0 the operator $U_{z_0}(z)$ is bounded and boundedly invertible.

The invertibility of $Q(z)+W$ can be *expressis verbis* proved as in Theorem 2.3 if one remembers that in the limit case $N = \infty$ for any Riesz basis, in particular for $\{g_n(z)\}_{n=1}^{\infty}$, Im $\neq 0$, the corresponding infinite Gram–Schmidt matrix generates a bounded, positive and boundedly invertible operator in $\mathfrak{l}_2$ (see, for example, [6]).

Suppose that there is a vector $h \in \mathcal{H}$ such that $R_1(z_0)h = 0$ for some non-real z_0. By (3.3), this means that

$$\begin{aligned} R(z_0)\, h \, (\in \mathcal{D}(A)) &= \sum_{m,n=1}^{N} \left([Q(z) + W]^{-1} \right)_{mn} (h, g_n(\bar{z_0}))\, g_m(z_0) \\ &= \sum_{m=1}^{N} \left\{ \sum_{n=1}^{N} \left([Q(z) + W]^{-1} \right)_{mn} (h, g_n(\bar{z_0})) \right\} g_m(z_0) \in \mathcal{N}. \end{aligned} \tag{3.5}$$

But for any $h \in \mathcal{H}$ the vector in the left-hand side of (3.5) belongs to $\mathcal{D}(A)$ while the corresponding vector in the right-hand side of (3.5) belongs to $\mathcal{N}$. However, by our assumptions $\mathcal{D}(A) \cap \mathcal{N} = \{0\}$. Hence both sides of (3.5) are zero-vectors, particularly $R(z_0)\, h = 0$. Recalling that the resolvent $R(z_0)$ of selfadjoint operator A is invertible, we conclude that $h = 0$.

The property $R_1(z)^* = R_1(\bar{z})$, Im$z \neq 0$ is evident.

The fact that $R_1(z)$ satisfies the Hilbert identity for any two non-real z_1, z_2 can be checked out by an elementary algebraic computation. □

The following theorem extends the class of singular perturbations of selfadjoint operators.

Theorem 3.2. *Let $\mathcal{H}$ and $\mathcal{K}$ be Hilbert spaces, A be an unbounded selfadjoint operator in $\mathcal{H}$ and $R(z)$,* Im$z \neq 0$, *is the resolvent of A, $G(z)$ is a bounded holomorphic in the open upper and lower half-planes operator function from $\mathcal{K}$ to $\mathcal{H}$ satisfying the conditions*

- *for any non-real z, z_0*

$$G(z) = G(z_0) + (z - z_0) R(z) G(z_0), \tag{3.6}$$

- *at least for one and hence for all non-real z zero is not an eigenvalue of the operator $G(z)^* G(z)$ and the intersection of the domain $\mathcal{D}(A)$ of A and the subspace $\mathcal{N} = \overline{G(z_0)\mathcal{K}} \subset \mathcal{H}$ consists only of the zero-vector;*

$Q(z)$ is a holomorphic in the open upper and lower half-planes operator function in $\mathcal{K}$ such that

- *$Q(z)^* = Q(\bar{z}),\ z \neq 0$;*

- *for any non-real* z, z_0

$$Q(z) - Q(z_0) = (z - z_0)G(\bar{z}_0)^* G(z). \tag{3.7}$$

Then for any invertible selfadjoint operator L *in* $\mathcal{K}$ *such that* L^{-1} *is compact the operator* $Q(z) + L$, $\mathrm{Im} z \neq 0$, *is invertible, has compact inverse and the operator function*

$$R_L(z) = R(z) - G(z) \left[Q(z) + L\right]^{-1} G(\bar{z})^* \tag{3.8}$$

is a resolvent of some selfadjoint operator A_1.

Proof. Suppose that for some non-real z_0 zero is not an eigenvalue of $G(z_0)^* G(z_0)$ and at the same time there are a non-real z_1 and a non-zero $h \in \mathcal{K}$ such that $G(z_1)h = 0$. Then by (3.6)

$$G(z_0)h = \left[I + (z_0 - z_1)R(z_0)\right] R(z_1)h = 0,$$

a contradiction.

By our assumptions for any non-real z zero is not an eigenvalue of the operator $Q(z) + L$. Indeed, suppose that for some h from the domain of L we have $\left[Q(z) + L\right] h = 0$. Then

$$0 = \mathrm{Im}\left(\left[Q(z) + L\right] h, h\right) = \mathrm{Im}\left(Q(z)^* Q(z)h, h\right).$$

But $Q(z)^* Q(z)$ is a non-negative invertible operator. Hence $h = 0$.

Since for non-real z, zero is not an eigenvalue of the operator $Q(z) + L$, by virtue of the invertibility of the operator L, compactness of L^{-1} and the obvious equality

$$Q(z) + L = L\left[L^{-1}Q(z) + I\right],$$

"–1" is not an eigenvalue of operator $L^{-1}Q(z)$. But $L^{-1}Q(z)$ is a compact operator. Therefore the operator $L^{-1}Q(z) + I$ is boundedly invertible [7] and so is the operator $Q(z) + L$,

$$\left[Q(z) + L\right]^{-1} = \left[L^{-1}Q(z) + I\right]^{-1} L^{-1}.$$

Obviously, the inverse of $Q(z) + L$ is a compact operator.

The fact that $R_1(z)$ is the resolvent of a self-adjoint operator is proved by the same arguments as above. □

4. Singular perturbations of selfadjoint Laplace operator. Null-range potentials

Let A be an unbounded selfadjoint operator. By a *regular* perturbation of A we call any selfadjoint operator A_1 defined as in Theorem 2.3. Following [3], we say that A_1 is a *singular* perturbation of A if A_1 is defined by A as in Theorem 3.1 or 3.2. In this section we will consider a special class of singular perturbations of the selfadjoint Laplace operator

$$-\Delta = -\frac{\partial^2}{\partial x_1^2} - \frac{\partial^2}{\partial x_2^2} - \frac{\partial^2}{\partial x_3^2}$$

in $\mathbf{L}_2(\mathbb{R}^3)$ defined on the Sobolev subspaces $H_2^2\left(\mathbb{R}^3\right)$, namely, the class of operators which fit into the conditions of Theorem 3.1. We will use here the symbol A to denote the specified unperturbed Laplace operator and the symbol $R(z)$ to denote the resolvent of A. Recall that

$$\left(R(z)f\right)(\mathbf{x}) = \frac{1}{4\pi}\int_{\mathbb{R}^3} \frac{e^{i\sqrt{z}|\mathbf{x}-\mathbf{x}'|}}{|\mathbf{x}-\mathbf{x}'|} f\left(\mathbf{x}'\right)d\mathbf{x}', \quad \mathrm{Im}\sqrt{z} > 0, \quad \mathbf{x} = (x_1, x_2, x_3)\,. \quad (4.1)$$

A simple, but fundamentally important example of singular perturbation of A was first rigorously examined in the short note [4] in the framework of the theory of self-adjoint extensions of symmetric operators. Actually, it was proved in [4] that for

$$g(z;\mathbf{x}) = \left(R(z)\delta\right)(\mathbf{x}) = \frac{1}{4\pi}\frac{e^{i\sqrt{z}|\mathbf{x}|}}{|\mathbf{x}|},$$

where $\delta\left(\mathbf{x}\right)$ is the Dirac δ-function, and for any real α the operator function

$$R_\alpha(z) = R(z) - \frac{1}{Q(z)+\alpha}\left(\cdot, g(\bar{z};\cdot)\right)g(z;\cdot), \quad Q(z) = \frac{i\sqrt{z}}{4\pi}, \quad (4.2)$$

is the resolvent of selfadjoint operator A_α. In accordance with (4.2), the domain $\mathcal{D}_\alpha$ of A_α consists of functions

$$f(\mathbf{x}) = f_0(\mathbf{x}) - \frac{1}{Q(z)+\alpha}\cdot f_0(\mathbf{0})\cdot g(z;\mathbf{x}), \quad (4.3)$$

where functions $f_0(\mathbf{x})$ run over the space H_2^2 and

$$\left(A_\alpha f\right)(\mathbf{x}) = \left(Af_0\right)(\mathbf{x}) - \frac{z}{Q(z)+\alpha}\cdot f_0(\mathbf{0})\cdot g(z;\mathbf{x}). \quad (4.4)$$

The expressions (4.3)–(4.4) are correct since any vector $\hat{f}_0$ of $H_2^2\left(\mathbb{R}^3\right)$ is equivalent to some Hölder-continuous function $f_0(\mathbf{x})$ with any index $\gamma < \frac{1}{2}$ [7], and consequently the product $|\mathbf{x}|\cdot f_0(\mathbf{x})$ is differentiable in $|\mathbf{x}|$ at $\mathbf{x} = \mathbf{0}$ and

$$\lim_{|\mathbf{x}|\downarrow 0}\frac{\partial}{\partial|\mathbf{x}|}\left(|\mathbf{x}|f(\mathbf{x})\right) = f_0(\mathbf{0}). \quad (4.5)$$

With account of (4.3) and (4.5) it can be argued that functions $f(\mathbf{x})$ from $\mathcal{D}_\alpha$ satisfies the "boundary condition"

$$\lim_{|\mathbf{x}|\downarrow 0}\left[\frac{\partial}{\partial|\mathbf{x}|}\left(|\mathbf{x}|f(\mathbf{x})\right) + 4\pi\alpha|\mathbf{x}|f(\mathbf{x})\right] = 0. \quad (4.6)$$

For real α the selfadjoint operator A_α legalizes the formal expression $-\Delta + (4\pi\alpha)^{-1'}\cdot\delta(\mathbf{x})$ and associated with A_α the condition (4.6) is said to be a zero-range potential [4, 2].

Note that the $g(z;\cdot)$ in (4.2) does not belong to $\mathcal{D}(A)$, otherwise the functional

$$\varphi(0) = -\int_{\mathbb{R}^3}\left[\left(\Delta\varphi\right)(\mathbf{x}) + z\varphi\left(\mathbf{x}\right)\right]\cdot g(\bar{z};\mathbf{x})d\mathbf{x} \quad (4.7)$$

would be bounded on the set of infinitely smooth compact function $\varphi(\mathbf{x})$. Besides,

$$(z-z_0)\,(g(z),g(\bar{z}_0)) = \lim_{|\mathbf{x}|\downarrow 0}\,[g(z;\mathbf{x})-g(z_0;\mathbf{x})] = Q(z)-Q(z_0).$$

Therefore the result from [4] is a special case of Theorem 3.1, where A is the standardly defined Laplace operator and $N=1$.

Referring to the conditions of Theorem 3.1, it is easy to check that the stated assertion about $R_\alpha(z)$ admits the following (in fact, well-known [2, 3]) generalization. Let

$$\begin{aligned} g_n(z;\mathbf{x}) &= R(z)\delta(\cdot-\mathbf{x}_n)(\mathbf{x}) = \frac{1}{4\pi}\frac{e^{i\sqrt{z}|\mathbf{x}-\mathbf{x}_n|}}{|\mathbf{x}-\mathbf{x}_n|}, \quad 1<n\le N<\infty; \\ Q(z) &= (q_{mn}(z))_{m,n=1}^{N} = \begin{cases} q_{mn}(z) = g_n(z;\mathbf{x}_m-\mathbf{x}_n), & m\neq n, \\ q_{mm}(z) = \frac{i\sqrt{z}}{4\pi}. \end{cases} \end{aligned} \tag{4.8}$$

Using the same arguments as above, it is easy to check that any non-zero linear combination of functions $g_n(z;\mathbf{x})$ does not belong to $\mathcal{D}(A)$. Besides, $Q(z)$ is a holomorphic in the open upper and lower half-planes infinite matrix function defining at each non-real z a bounded operator in the space $\mathbf{l}_2$ such that

- $Q(z)^* = Q(\bar{z}),\ \text{z}\neq 0;$
- for any non-real z, z_0

$$Q(z)-Q(z_0) = (z-z_0)\left((g_m(z),g_n(\bar{z}_0))\right)^T_{1\le m,n<\infty}\,. \tag{4.9}$$

As follows by Theorem 3.1, for any invertible Hermitian matrix $W=(w_{mn})_{m,n=1}^{N}$ the operator function

$$R_\alpha(z) = R(z) - \sum_{m,n=1}^{N}\left([Q(z)+W]^{-1}\right)_{mn}(\cdot,g_n(\bar{z};\cdot))\,g_m(z;\cdot) \tag{4.10}$$

is the resolvent of the selfadjoint operator A_W in $\mathbf{L}_2(\mathbb{R}^3)$.

Let us denote by $\mathcal{N}$ the linear span of functions $\{g_n(z;\mathbf{x})\}$. The operator A_W is, loosely speaking, the Laplace differential operator $-\Delta$ with the domain

$$\begin{aligned} \mathcal{D}_W := \{ f : f = f_0 + g,\ f\in H_2^2\left(\mathbb{R}^3\right), g\in\mathcal{N}, \\ \lim_{\rho_m\to 0}\left[\frac{\partial}{\partial\rho_m}(\rho_m f(\mathbf{x}))\right] + \sum_{n=1}^{N} 4\pi\cdot w_{mn}\lim_{\rho_n\to 0}[\rho_n f(\mathbf{x})] = 0, \\ \rho_n = |\mathbf{x}-\mathbf{x}_n|, \quad 1\le n\le N\}\,. \end{aligned} \tag{4.11}$$

If the matrix W is diagonal, that is, $w_{mn}=\alpha_m\cdot\delta_{mn}$, then A_W is the Laplace operator perturbed by a collection of "zero-range" potentials

$$\lim_{\rho_m\to 0}\left[\frac{\partial}{\partial\rho_m}(\rho_m f(\mathbf{x})) + 4\pi\alpha_m\cdot\rho_m f(\mathbf{x})\right] = 0.$$

Under some conditions, the last statements remain true also in the case of the infinite set of points $\{\mathbf{x}_n\}_{-\infty}^{\infty}$. Let the set of functions $g_n(z;\mathbf{x})$ and infinite matrix function $Q(z)$ be like in (4.8) and $\mathcal{N}$ denotes the closed linear span of functions $g_n(z;\mathbf{x})$.

Theorem 4.1 (A. Grossmann, R. Høegh-Krohn, M. Mebkhout). *If*

$$\inf_{-\infty<m,n<\infty} |\mathbf{x}_m - \mathbf{x}_n| = d > 0,$$

then for a selfadjoint operator in $\mathbf{l}_2$ *defined by the infinite matrix*

$$W = (w_{mn})_{m,n=-\infty}^{\infty},$$

the operator function

$$R_W(z) = R(z) - \sum_{m,n=-\infty}^{\infty} \left([Q(z)+W]^{-1}\right)_{mn} (\cdot, g_n(\bar{z};\cdot))\, g_m(z;\cdot)$$

is the resolvent of selfadjoint operator $-\Delta_W$ *in* $\mathbf{L}_2(\mathbb{R}^3)$, *which is the Laplace operator with the domain*

$$\begin{aligned}\mathcal{D}_W := \big\{ f :\ & f = f_0 + g,\ f_0 \in H_2^2\left(\mathbb{R}^3\right),\ g \in \mathcal{N}, \\ & \lim_{\rho_m \to 0} \left[\frac{\partial}{\partial \rho_m}\left(\rho_m f(\mathbf{x})\right)\right] + \sum_{n=-\infty}^{\infty} w_{mn} \lim_{\rho_n \to 0} [\rho_n f(\mathbf{x})] = 0, \\ & \rho_n = |\mathbf{x} - \mathbf{x}_n|, \quad -\infty \le n < \infty \big\}.\end{aligned}$$

Theorem 4.1 is a direct consequence of Theorem 3.1 and the following proposition.

Proposition 4.2. *If*

$$\inf_{m,n} |\mathbf{x}_m - \mathbf{x}_n| = d > 0 \tag{4.12}$$

and $\operatorname{Im} z \neq 0$, *then* $Q(z)$ *is the matrix of a bounded operator in the natural basis of* $\mathbf{l}_2$ *and the sequence of* $\mathbf{L}_2(\mathbb{R}^3)$*-vectors* $\{g_n(z;\cdot)\}_1^\infty$ *is the Riesz basis in its closed linear span* $\mathcal{N}$.

Proof. By (4.8) and (4.12), for $\operatorname{Im}\sqrt{z} = \eta + i\kappa$ with $\kappa > 0$ we see that

$$\sum_n |q_{mn}(z)| \le \frac{\sqrt{\eta^2+\kappa^2}}{4\pi} + \frac{1}{4\pi d} \sum_{n\neq m} e^{-\kappa|\mathbf{x}_n - \mathbf{x}_m|} < \infty.$$

and noting that there are at most $3n^2 + \frac{1}{4}$ points $\mathbf{x}_n$ in the spherical layer $(n-\frac{1}{2})d \le |\mathbf{x} - \mathbf{x}_m| < (n+\frac{1}{2})$, $n \ge 1$, we obtain that

$$\begin{aligned}\sum_{n\neq m} e^{-\kappa|\mathbf{x}_n - \mathbf{x}_m|} &\le \frac{13}{4} e^{-\kappa d} + \sum_2^\infty \left(3n^2 + \frac{1}{4}\right) e^{-\left(n-\frac{1}{2}\right)\kappa d} \\ &\le \frac{13}{4} e^{-\kappa d} + O\left(e^{-\frac{3}{2}\kappa d}\right) \quad (\text{as } \kappa \to \infty).\end{aligned} \tag{4.13}$$

Hence for non-real z,

$$M(z) = \sup_m \sum_n |q_{mn}(z)| < \infty,$$

and the infinite matrix $Q(z)$ generates a bounded operator in $\mathbf{l}_2$ with the norm $\|Q(z)\| \le M(z)$.

As it was mentioned in the proof of Theorem 3.1, in order to establish that for any regular point z of the Laplace operator A the set of $\mathbf{L}_2(\mathbb{R}^3)$-functions $\{g_n(z) = g(z; \mathbf{x} - \mathbf{x}_n)\}$ forms a Riesz basis in its linear span, it suffices to verify this for at least one such point, say for a point $-\kappa^2$, where κ is a sufficiently large positive number. For $z = -\kappa^2$ the Gram–Schmidt matrix for the set of functions $\{g_n(-\kappa^2)\}$ has form

$$\Gamma(-\kappa^2) = \frac{1}{8\pi\kappa} \left(e^{-\kappa|\mathbf{x}_m - \mathbf{x}_n|} \right)_{-\infty}^{\infty}. \tag{4.14}$$

By (4.14) the matrix $8\pi\kappa \cdot \Gamma(-\kappa^2)$ is the sum $I + \Delta(-\kappa^2)$ of the infinite unity matrix I and the matrix $\Delta(-\kappa^2)$, which according to (4.13) generates a bounded operator in $\mathbf{l}_2$ with norm of less than one for sufficiently large κ. Therefore the matrix $\Gamma(-\kappa^2)$ generates a bounded and boundedly invertible operator in $\mathbf{l}_2$. Hence vectors $\{g_n(-\kappa^2)\}$ form a Riesz basis in their linear span. □

5. Singular perturbations of selfadjoint Laplace operator. 1D-located perturbation

We describe further a special class of singular selfadjoint perturbations of the Laplace operator A falling under the conditions of Theorem 3.2. In the cases discussed below, $\mathbf{L}_2(\mathbb{R}^3)$ plays naturally the role of Hilbert space $\mathcal{H}$, the usual space $\mathbf{L}_2([0, l])$ of square integrable functions on the interval $[0, l]$ with $l < \infty$ appears as the Hilbert space $\mathcal{K}$ wherein this interval itself is identified with the subset $\mathfrak{l} = \{0 \le x_1 \le l,\ x_2 = 0,\ x_3 = 0\}$ of $\mathbb{R}^3$. We define the holomorphic operator function $G(z)$, $\mathrm{Im}(z) \ne 0$ from $\mathbf{L}_2([0, l])$ to $\mathbf{L}_2(\mathbb{R}^3)$ setting

$$\begin{aligned} (G(z)u)(\mathbf{x}) &= \int_0^l g(z|x_1, x_2, x_3; x_1', 0, 0)\, u(x_1') dx_1', \quad u(\cdot) \in \mathbf{L}_2([0, l]), \\ g(z|x_1, x_2, x_3; x_1', x_2', x_3') &= g(z|\mathbf{x}, \mathbf{x}') = \frac{1}{4\pi} \frac{e^{i\sqrt{z}|\mathbf{x} - \mathbf{x}'|}}{|\mathbf{x} - \mathbf{x}'|}, \quad \mathrm{Im}\sqrt{z} > 0. \end{aligned} \tag{5.1}$$

It follows from (5.1) that

$$|(G(z)u)(\mathbf{x})|^2 \le \int_0^l |g(z|x_1 - x_1', x_2, x_3; 0, 0, 0)|^2 \, dx_1' \cdot \|u\|^2 .$$

Therefore for $z \ne 0$, the operator $G(z)$ is bounded and

$$\|G(z)\| \le \frac{1}{\sqrt{8\pi \mathrm{Im}\sqrt{z}}}. \tag{5.2}$$

Note that the Fourier transform

$$\widehat{G(z)u}\,(k_1,k_2,k_3) = \frac{1}{2\pi}\cdot\frac{1}{k_1^2+k_2^2+k_3^2-z}\hat{u}(k_1)$$

of $G(z)u(\mathbf{x})$, where

$$\hat{u}(k_1) = \frac{1}{\sqrt{2\pi}}\int\limits_0^l e^{-ik_1x_1}u(x_1)dx_1,$$

equals to zero if and only if $\hat{u}(k_1)\equiv 0$ and as follows $u(x_1)=0$ almost everywhere on $[0,l]$. Accordingly, $G(z)u(\cdot)=0$ *in* $\mathbf{L}_2(\mathbb{R}^3)$ *if and only if* $u(\cdot)=0$ *in* $\mathbf{L}_2([0,l])$. Therefore for any non-real z zero is not an eigenvalue of $G(z)^*G(Z)$. We note that the adjoint operator $G(z)^*$ from $\mathbf{L}_2(\mathbb{R}^3)$ to $\mathbf{L}_2([0,l])$ is determined by the formula

$$\left(G(z)^*f\right)(x) = \int_{\mathbb{R}^3} g(\bar{z}|x,0,0;\mathbf{x}')f(\mathbf{x}')d\mathbf{x}',\quad f(\cdot)\in\mathbf{L}_2(\mathbb{R}^3),\ x\in[0,\mathfrak{l}], \tag{5.3}$$

which makes sense, since the functions

$$f(\mathbf{x}) = \int_{\mathbb{R}^3} g(\bar{z}|\mathbf{x};\mathbf{x}')w(\mathbf{x}')d\mathbf{x}',\quad w(\cdot)\in\mathbf{L}_2(\mathbb{R}^3),\quad \mathrm{Im}z\neq 0,$$

forming the domain $\mathcal{D}(A)$ of A are continuous [7].

Suppose further that there is a vector $h\in\mathbf{L}_2(\mathbb{R}^3)$ from the subspace $\mathcal{N} = \overline{G(z)\mathbf{L}_2([0,l])}$ that belongs to the domain $\mathfrak{D}(A)$ of the Laplace operator A. h as any vector from $\mathfrak{D}(A)$ can be represented in the form $h=R(z)w$ with some $w\in\mathbf{L}_2(\mathbb{R}^3)$ while by our assumption there is a sequence of vectors $\{u_n\in\mathbf{L}_2([0,l])\}$ such that

$$\lim_{n\to\infty}\|R(z)w - G(z)u_n\|_{\mathbf{L}_2(\mathbb{R}^3)} = 0. \tag{5.4}$$

Now recall that for each $w\in\mathbf{L}_2(\mathbb{R}^3)$ and any $\varepsilon>0$ it is possible to find an infinitely smooth compact function $\phi(\mathbf{r})$ which is also equal to zero at some neighborhood of the subset $\mathfrak{l}$ to satisfy the condition

$$\left|(w,\phi)_{\mathbf{L}_2(\mathbb{R}^3)}\right| \geq (1-\varepsilon)\,\|w\|^2_{\mathbf{L}_2(\mathbb{R}^3}\,. \tag{5.5}$$

Taking into account further that for $\phi(\mathbf{r})$, as well as for any smooth compact function,

$$\phi(\mathbf{r}) = \frac{1}{4\pi}\int_{\mathbb{R}^3}\frac{e^{i\sqrt{z}|\mathbf{x}-\mathbf{x}'|}}{|\mathbf{x}-\mathbf{x}'|}\left[-\Delta\phi\left(\mathbf{x}'\right) - z\phi\left(\mathbf{x}'\right)\right]d\mathbf{x}', \tag{5.6}$$

we notice that

$$\begin{aligned}(G(z)w,[-\Delta\phi-\bar{z}\phi])_{\mathbf{L}_2(\mathbb{R}^3)} &= (w,\phi)_{\mathbf{L}_2(\mathbb{R}^3)}\,,\\ (G(z)u,[-\Delta\phi-\bar{z}\phi])_{\mathbf{L}_2(\mathbb{R}^3)} &= 0,\quad u\in\mathbf{L}_2([0,l]).\end{aligned}$$

Hence for the above sequence $\{u_n \in \mathbf{L}_2([0,l])\}$ by virtue of (5.5) we conclude that

$$\begin{aligned} &\|R(z)w - G(z)u_n\|_{\mathbf{L}_2(\mathbb{R}^3)} \cdot \|-\Delta\phi - \bar{z}\phi\|_{\mathbf{L}_2(\mathbb{R}^3)} \\ &\geq \left|\left([R(z)w - G(z)u_n], [-\Delta\phi - \bar{z}\phi]\right)_{\mathbf{L}_2(\mathbb{R}^3)}\right| \\ &= \left|(w,\phi)_{\mathbf{L}_2(\mathbb{R}^3)}\right| \geq (1-\varepsilon)\|w\|^2_{\mathbf{L}_2(\mathbb{R}^3)} . \end{aligned} \tag{5.7}$$

But in view of (5.4) for $n \to \infty$ the last inequality in (5.7) must necessarily be violated unless $w = 0$. Therefore $\mathcal{N} \cap \mathfrak{D}(A) = \{0\}$.

In accordance with our choice (5.1) of the mapping $G(z)$, the bounded holomorphic operator function $Q(z)$ in $\mathbf{L}_2([0,l])$ in the corresponding Theorem 3.2 may be determined by setting

$$\begin{aligned} (Q(z)u)(x) &= \int_0^l q(z|x,x')u(x')dx' \\ &\equiv \frac{1}{4\pi}\int_0^l \frac{e^{i\sqrt{z}|x-x'|}-1}{|x-x'|}u(x')dx', \quad u \in \mathbf{L}_2([0,l]),\ \mathrm{Im}\sqrt{z} > 0. \end{aligned} \tag{5.8}$$

Since the kernel $q(z|x,x')$ of integral operator $Q(z)$ is a continuous function on the set $[0,l]\times[0,l]$, then for any non-positive z the operator $Q(z)$ is bounded and moreover compact.

For the operator function $Q(z)$ defined by the expression (5.8) the property $Q(z)^* = Q(\bar{z})$ is obvious and the relation (3.6) follows immediately from the Hilbert identity for the resolvent kernel of the Laplace operator A:

$$g(z|\mathbf{x},\mathbf{x}') - g(z_0|\mathbf{x},\mathbf{x}') = (z-z_0)\int_{\mathbb{R}^3} g(z_0|\mathbf{x},\mathbf{x}'')g(z|\mathbf{x}'',\mathbf{x}')d\mathbf{x}'', \quad \mathrm{Im}z_0,\ \mathrm{Im}z \neq 0.$$

in cases where $\mathbf{x} = (x_1 = x, x_2 = 0, x_3 = 0)$, $\mathbf{x}' = (x_1 = x', x_2 = 0, x_3 = 0)$.

Finally, in the case under consideration we can take as L in (3.8) the selfadjoint Sturm–Liouville operator

$$L = -\frac{d^2}{dx^2} + \mathfrak{v}(x)$$

in $\mathbf{L}_2([0,l])$ with a real continuous "potential" $\mathfrak{v}(x)$ assuming that the domain $\mathcal{D}(L)$ of L consists of functions $u(x)$ from the Sobolev class $H_2^2([0,l])$ satisfying the boundary conditions $u(0) = u(l) = 0$. We confine ourselves also to only those potentials $\mathfrak{v}(x)$ for which zero is not an eigenvalue of the operator L. Since the concerned Sturm–Liouville operators are semi-bounded from below, have simple discrete spectrum and for their eigenvalues λ_n numbered in increasing order, we have the relation

$$\lambda_n \underset{n\to\infty}{=} \frac{\pi^2 n^2}{l^2}\left[1 + O\left(\frac{1}{n}\right)\right],$$

then L^{-1} is a compact operator of trace class.

Thus, the related to the Laplace operator operator A operator functions $G(z)$ and $Q(z)$ and defined by formulas (5.1) and (5.8), respectively and the introduced selfadjoint Sturm–Liouville operator L in $\mathbf{L}_2([0,l])$ satisfy all the conditions of Theorem 3.2. Hence, the operator function $R_L(z)$ defined by the expression (3.8) is the resolvent of some singular perturbation A_L of A in $\mathbf{L}_2(\mathbb{R}^3)$.

Proposition 5.1. *Any smooth compact function $\phi(\mathbf{r})$, which is equal to zero at some neighborhood of the subset $\mathfrak{l}$ belongs to $\mathcal{D}(A_L)$ and*

$$(A_L\phi)(\mathbf{r}) = (A\phi)(\mathbf{r}) = -\Delta\phi(\mathbf{r}).$$

Proof. By virtue of (5.3), the identity (5.6) and the assumptions of the proposition

$$(G(\bar{z})^*[-\Delta\phi - z\phi])(x) = \phi(x,0,0) = 0, \quad x \in [0,l].$$

In accordance with (3.8), this means that

$$(R_L(z)[-\Delta\phi - z\phi])(\mathbf{r}) = (R(z)[-\Delta\phi - z\phi])(\mathbf{r}) = \phi(\mathbf{r}). \tag{5.9}$$

Therefore $\phi \in \mathcal{D}(A_L) \cap \mathcal{D}(A)$ and, in view of (5.9),

$$\begin{aligned}(A_L\phi)(\mathbf{r}) &= -\Delta\phi(\mathbf{r}) - z\phi(\mathbf{r}) + z\,(R_L(z)[-\Delta\phi - z\phi])(\mathbf{r})\\ &= -\Delta\phi(\mathbf{r}) - z\phi(\mathbf{r}) + z\phi(\mathbf{r}) = -\Delta\phi(\mathbf{r}).\end{aligned}$$ □

Proposition 5.2. *Let $f(x_1,x_2,x_3)$ be a function from $\mathcal{D}(A_L)$ and $u_f(x)$, $x \in [0,l]$, be defined by*

$$u_f(x) = -\lim_{\rho\to 0}\frac{1}{\ln(\rho^2)}f(x,x_2,x_3), \quad \rho = \sqrt{x_2^2 + x_3^2}.$$

Then $u_f \in \mathcal{D}(L)$ and

$$\begin{aligned}(Lu_f)(x) = -4\pi\cdot\lim_{\rho\to 0}\Bigg[& f(x,x_2,x_3) + \ln\left(\frac{1}{\rho^2}\right)\cdot u_f(x)\\ & +2\ln 2\cdot u_f(x) - \int_0^l \frac{s-x}{|s-x|}\ln|s-x|u_f'(s)ds\Bigg].\end{aligned}$$

Proof. Turning to the expressions (3.8) and (5.3), we recall first of all that the functions from $\mathcal{D}(A)$ are continuous [7]. Therefore for any $h(\mathbf{x})$ from $\mathbf{L}_2(\mathbb{R}^3)$ the functions $(R(z)h)$ and $(G(z)^*h)(x)$ from $\mathbf{L}_2(\mathbb{R}^3)$ and $\mathbf{L}_2([0,l])$, respectively, are continuous. We also take into account that the domains of operators L and $L+Q(z)$ coincide, since $Q(z)$ is a bounded operator. By our assumptions "0" is a regular point of operator $L+Q(z)$, $\mathrm{Im}z \neq 0$. Therefore for any $h \in \mathbf{L}_2(\mathbb{R}^3)$ the function

$$\hat{u}_h(x) = \left([L+Q(z)]^{-1}G(z)^*h\right)(x)$$

belongs to $\mathcal{D}(L)$, that is, to the Sobolev class $H_2^2([0,l])$ and satisfies the boundary conditions $\hat{u}_h(0) = \hat{u}_h(l) = 0$.

Writing any $f \in \mathcal{D}(A_L)$ in the form $f(\mathbf{x}) = (R_L(z)h)(\mathbf{x})$ with some $h \in \mathbf{L}_2(\mathbb{R}^3)$ we can find the limiting value of $(R_L(z)h)(\mathbf{x})$, when $\rho = \sqrt{x_2^2 + x_3^2} \to 0$

and $x_1 \in [0,l]$ using the following elementary assertion, the proof of which are left to the reader.

Lemma 5.3. *Let $u(x)$ be continuously differentiable function on $[0,l]$ satisfying the conditions $u(0)=u(l)=0$. Then*

$$\int_0^l \frac{1}{\sqrt{(x-s)^2+\rho^2}} u(s)ds \underset{\rho\to 0}{=} u(x)\cdot \ln\frac{1}{\rho^2} + 2\ln 2u(x) - \int_0^l \frac{s-x}{|s-x|}\ln|s-x|\, u'(s)\, ds.$$

Using the expression (3.8) for $(R_L(z)h)(\mathbf{x})$ and applying Lemma 5.3 one can easily verify that

$$u_f(x) = -\lim_{\rho\downarrow 0}\frac{1}{\ln(\rho^2)} f(x,x_2,x_3) = -\frac{1}{4\pi}\hat{u}_h(x) \in \mathcal{D}(L)$$

and

$$\begin{aligned}
&\lim_{\rho\downarrow 0}\Bigg[f(x,x_2,x_3) + \ln\left(\frac{1}{\rho^2}\right)\cdot u_f(x) \\
&\quad + 2\ln 2\cdot u_f(x) - \int_0^l \frac{s-x}{|s-x|}\ln|s-x|\, u_f'(s)\, ds\Bigg] \\
&= (G(z)^*h) - \Big(Q(z)\,[L+Q(z)]^{-1}\, G(z)^*h\Big)(x) \\
&= L\Big([L+Q(z)]^{-1}\, G(z)^*h\Big)(x) = L\hat{u}_h(x) = -\frac{1}{4\pi}(Lu_f)(x).
\end{aligned}$$

□

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Generic asymptotics of resonance counting function for Schrödinger point interactions

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Abstract. We study the leading coefficient in the asymptotic formula $\mathcal{N}(R) = \frac{W}{\pi}R + O(1)$, $R \to \infty$, for the resonance counting function $\mathcal{N}(R)$ of Schrödinger Hamiltonians with point interactions. For such Hamiltonians, the Weyl-type and non-Weyl-type asymptotics of $\mathcal{N}(R)$ was introduced recently in a paper by J. Lipovský and V. Lotoreichik (2017). In the present paper, we prove that the Weyl-type asymptotics is generic.

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Keywords. asymptotics of resonances, delta-interaction, directed graph, multigraph, exponential polynomial, quasi-normal-eigenvalue, Weyl-type asymptotics.

This work is dedicated to the dear Memory of Boris Pavlov. The first author had the great experience to meet him personally at a conference in Dubna back in 1987. At that time Boris was developing his original approach to point interactions and was the leader of a very strong group of young enthusiastic mathematicians working in this area. From then on our steady friendship developed, with him and his coworkers. The authors are very grateful to Boris for the many insights he has provided, that also influenced much of our work. We deeply mourn his departure.

1. Introduction

The asymptotics as $R \to \infty$ of the counting function $\mathcal{N}_{H_{a,Y}}(R)$ for the resonances of a "one particle, finitely many centers" Schrödinger Hamiltonian $H_{a,Y}$ acting in the complex Lebesgue space $L^2(\mathbb{R}^3)$ and associated with the formal differential

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expression

$$-\Delta u(x) + \text{“}\sum_{j=1}^{N} \mu(a_j)\delta(x-y_j)u(x)\text{”}, \quad x=(x^1,x^2,x^3)\in\mathbb{R}^3,\ N\in\mathbb{N}, \tag{1.1}$$

have being studied recently in [25], where the existence of Weyl-type and non-Weyl type asymptotics of $\mathcal{N}_{H_{a,Y}}(\cdot)$ have been proved and similarities with the case of quantum graphs [12, 13] have been noticed. The goal of the present paper is to show that the case of Weyl-type asymptotics of $\mathcal{N}_{H_{a,Y}}(\cdot)$ is generic for operators of the form (1.1).

We denote by Δ the self-adjoint Laplacian in $L^2(\mathbb{R}^3)$ and assume throughout the paper that $N \geq 2$, where N is the number of point interaction *centers* $y_j \in \mathbb{R}^3$, which are assumed to be distinct, i.e., $y_m \neq y_j$ if $m \neq j$. The N-tuple of centers $(y_j)_{j=1}^N \subset (\mathbb{R}^3)^N$ is denoted by Y. The numbers $a_j \in \mathbb{C}$ are the “strength” parameters for the point interactions forming a tuple $a=(a_j)_{j=1}^N \in \mathbb{C}^N$.

Roughly speaking, point interactions correspond to potentials expressed by the Dirac measures $\delta(\cdot - y_j)$ and play the role of potentials in formula (1.1) (this can be taken as definition in the 1-D case of Sturm–Liouville differential operators). Rigorously, in 3-D case, the point interaction Hamiltonian $H_{a,Y}$ associated with (1.1) can be introduced as a densely defined closed operator in the Hilbert space $L^2(\mathbb{R}^3)$ via a Krein-type formula for the difference $(H_{a,Y}-z^2)^{-1}-(-\Delta-z^2)^{-1}$ of the perturbed and unperturbed resolvents of operators $H_{a,Y}$ and $-\Delta$, respectively. For the definition of $H_{a,Y}$ and for the meaning of the “strength” parameters and the factors $\mu(a_j)$ in (1.1), we refer to [1, 2, 3, 7] in the case $a_j \in \mathbb{R}$, and to [4, 6] in the case $a_j \notin \mathbb{R}$ (see also Sect. 2). Note that, in the case $(a_j)_{j=1}^N \subset \mathbb{R}^N$, the operator $H_{a,Y}$ is self-adjoint in $L^2(\mathbb{R}^3)$; and in the case $(a_j)_{j=1}^N \subset (\overline{\mathbb{C}_-})^N$, $H_{a,Y}$ is closed and maximal dissipative (in the sense of [16], or in the sense that $\mathrm{i}H_{a,Y}$ is maximal accretive [23]).

Eigenvalues and (continuation) resonances k of the corresponding operator $H_{a,Y}$ are connected with the special $N \times N$-matrix $\Gamma(z)$, which is a function of the spectral parameter z and depends also on Y and a. The matrix-function $\Gamma(\cdot)$ appears naturally as a part of the expression for $(H_{a,Y}-z^2)^{-1}-(-\Delta-z^2)^{-1}$, see [3, 5, 6] and Sect. 2. The set $\Sigma(H_{a,Y})$ of resonances associated with $H_{a,Y}$ is defined as the set of zeroes k of the determinant $\det\Gamma(\cdot)$, which is an analytic of z function.

This definition follows the logic of [15, 12, 25] and slightly differs from that of the original definition [3, 5] since it includes in the set of resonances the zeroes $k \in \mathbb{C}_+ := \{z \in \mathbb{C} : \operatorname{Im} z > 0\}$, which correspond to eigenvalues k^2 of H_Y. It is easy to see [3, 5, 6] that $H_{a,Y}$ has only a finite number of eigenvalues and so the inclusion of corresponding $k \in \mathbb{C}_+$ does not essentially influence the asymptotics for $R \to \infty$ of the counting function $\mathcal{N}_{H_{a,Y}}(\cdot)$, which is defined by

$$\mathcal{N}_{H_{a,Y}}(R) := \#\{k \in \Sigma(H_{a,Y}) : |k| < R\}.$$

Here $\#E$ is the number of elements of a multiset E.

When the number of resonances in a certain domain is counted, $\Sigma(H_{a,Y})$ has to be understood as a multiset, i.e., an unordered set in which an element e can be repeated a finite number $m_e \in \mathbb{N}$ of times (this number m_e is called the multiplicity of e). The multiplicity of a resonance k is, by definition, its multiplicity as a zero of $\det \Gamma(\cdot)$, and it is always finite since the resolvent set of $H_{a,Y}$ is nonempty (see [3, 6]). The definition of the resonance counting function takes this multiplicity into account.

The investigation of the counting function $\mathcal{N}_{-\Delta+V}(\cdot)$ for scattering poles of Schrödinger Hamiltonians $-\Delta + V$ in $L^2(\mathbb{R}^n)$ with odd $n \geq 3$ was initiated in [26] (for the relation between the notions of scattering poles and resonances, see [15]). This study was continued and extended to obstacle and geometric scattering in a number of papers (see, e.g., [30, 18, 10, 11, 15, 31] and references therein). In particular, it was proved in [10, 11] that for odd $n \geq 3$ the formula

$$\limsup_{R\to\infty} \frac{\log \mathcal{N}_{-\Delta+V}(R)}{\log R} = n \tag{1.2}$$

is generic for compactly supported L^∞-potentials V. Generally, in such settings, only the bound $\limsup_{R\to\infty} \frac{\log \mathcal{N}_{-\Delta+V}(R)}{\log R} \leq n$ is proved [30] (see the discussion of a related open problem in [10, 31]).

During the last two decades, wave equations, resonances, and related optimization problems on structures with combinatorial geometry and graph theory backgrounds have attracted a substantial attention, in particular, due to their engineering applications, see monographs [3, 7, 8, 27], papers [6, 12, 13, 14, 17, 20, 21, 22] and references therein. One of the earliest studies of scattering on graphs was done by Gerasimenko and Pavlov [19].

In [13, 12], the asymptotics $\mathcal{N}_{\mathfrak{G}}(R) = \frac{2W_{\mathfrak{G}}}{\pi} R + O(1)$ as $R \to \infty$ for the resonance counting function of a non-compact quantum graph $\mathfrak{G}$ have been obtained and it was shown that the nonnegative constant $W_{\mathfrak{G}}$, which was called *the effective size of the graph*, is less or equal to the sum of lengths of the internal edges of the graph. It was said that the quantum graph has a Weyl resonance asymptotics if $W_{\mathfrak{G}}$ equals the sum of lengths of internal edges. Special attention was paid in [12, 13] to the cases where non-Weyl asymptotics holds, i.e., to the cases where $W_{\mathfrak{G}}$ is strictly less than the sum of lengths of internal edges.

In the recent paper [25], it was noticed that the resonance theories for point interactions and for quantum graphs have a lot in common, and the asymptotics

$$\mathcal{N}_{H_{a,Y}}(R) = \frac{W(H_{a,Y})}{\pi} R + O(1) \text{ as } R \to \infty \tag{1.3}$$

was established for point interaction Hamiltonians $H_{a,Y}$ with a certain positive constant $W(H_{a,Y})$, which is called *an effective size of the set* Y. (Note that (1.3) holds for the case $N \geq 2$; in the simple case $N = 1$ it is obvious that only one resonance exists.) On the other hand, *the size of the family of centers* Y was defined by

$$V(Y) := \max_{\sigma \in S_N} \sum_{j=1}^{N} |y_j - y_{\sigma(j)}|,$$

where the maximum is taken over all permutations σ in the symmetric group S_N. The asymptotics of $\mathcal{N}_{H_{a,Y}}(R)$ for $R \to \infty$ was called of *Weyl-type if the effective size* $W(H_{a,Y})$ *in* (1.3) *coincides with the size* $V(Y)$. An example of $H_{a,Y}$ with non-Weyl-type asymptotics was constructed in [25]. (Note that, while [25] considers only the case where all a_j coincide and are real, the results and proofs of [25] can be extended to the case of arbitrary $a \in \mathbb{C}^N$ almost without any changes.)

The present paper studies how often the equality $W(H_{a,Y}) = V(Y)$, i.e., Weyl-type asymptotics, happens. To parametrize rigorously the family of Hamiltonians $H_{a,Y}$, let us consider Y as a vector in the space $(\mathbb{R}^3)^N$ of ordered N-tuples $y = (y_j)_{j=1}^N$ with the entries $y_j \in \mathbb{R}^3$. We consider $(\mathbb{R}^3)^N$ as a linear normed space with the ℓ^2-norm $|y|_2 = (\sum |y_j|^2)^{1/2}$. Then the ordered collection Y of centers is identified with an element of the subset $\mathbb{A} \subset (\mathbb{R}^3)^N$ defined by

$$\mathbb{A} := \{y \in (\mathbb{R}^3)^N : y_j \neq y_{j'} \quad \text{for} \quad j \neq j'\}.$$

We consider $\mathbb{A}$ as a metric space with the distance function induced by the norm $|\cdot|_2$.

The following theorem is the main result of the present paper. It shows that Weyl-type asymptotics is generic for point interaction Hamiltonians and gives a precise sense to this statement.

Theorem 1.1. *There exists a subset* $\mathbb{A}_1 \subset \mathbb{A}$ *that is open and dense in the metric space* $\mathbb{A}$ *and has also the property that, for every* $Y \in \mathbb{A}_1$ *and every* $a \in \mathbb{C}^N$*, the counting function for the resonances of* $H_{a,Y}$ *has the Weyl-type asymptotics* $\mathcal{N}_{H_{a,Y}}(R) = \frac{V(Y)}{\pi} R + O(1)$ *as* $R \to \infty$.

The proof is constructive and is given in Sect. 3.2.

Notation. The following standard sets are used: the lower and upper complex half-planes $\mathbb{C}_\pm = \{z \in \mathbb{C} : \pm \operatorname{Im} z > 0\}$, the set $\mathbb{Z}$ of integers, the closure $\bar{S}$ of a subset of a normed space U, in particular, $\overline{\mathbb{C}}_\pm = \{z \in \mathbb{C} : \pm \operatorname{Im} z \geq 0\}$, open balls $\mathbb{B}_\epsilon(u_0) = \mathbb{B}_\epsilon(u_0; U) := \{u \in U : \rho_U(u, u_0) < \epsilon\}$ in a metric space U with the distance function $\rho_U(\cdot, \cdot)$ (or in a normed space).

By $y_j \sim y_m$ we denote an edge between vertices y_j and y_m in an undirected graph $\mathcal{G}$ (so $y_j \sim y_m$ and $y_m \sim y_j$ is the same edge). Directed edges in a directed graph $\overrightarrow{\mathcal{G}}$ will be called bonds in accordance with [8] and denoted by $y_j \rightsquigarrow y_m$, which means that the bond is from y_j to y_m (note that this notation is slightly different from that of [8]).

2. Resonances as zeroes of a characteristic determinant

Let the set $Y = \{y_j\}_{j=1}^N$ consist of $N \geq 2$ distinct points y_1, ..., y_N in $\mathbb{R}^3$. Let $a = (a_j)_{j=1}^N \in \mathbb{C}^N$ be the N-tuple of the strength parameters. The operator H

associated with (1.1) is defined in [1, 2, 3] for the case of real a_j, and in [6] for $a_j \in \mathbb{C}$. It is a closed operator in the complex Hilbert space $L^2(\mathbb{R}^3)$ and it has a nonempty resolvent set. The spectrum of H consists of the essential spectrum $[0, +\infty)$ and an at most finite set of points outside of $[0, +\infty)$ [6] (all of those points are eigenvalues).

The resolvent $(H - z^2)^{-1}$ of H is defined in the classical sense on the set of $z \in \mathbb{C}_+$ such that z^2 is not in the spectrum, and has the integral kernel

$$(H - z^2)^{-1}(x, x') = G_z(x - x') + \sum_{j,j'=1}^{N} G_z(x - y_j) \, [\Gamma_{a,Y}]^{-1}_{j,j'} \, G_z(x' - y_{j'}), \quad (2.1)$$

where $x, x' \in \mathbb{R}^3 \setminus Y$ and $x \neq x'$; see, e.g., [3, 6]. Here

$$G_z(x - x') := \frac{e^{\mathrm{i}z|x-x'|}}{4\pi|x - x'|}$$

is the integral kernel associated with the resolvent $(-\Delta - z^2)^{-1}$ of the kinetic energy Hamiltonian $-\Delta$; $[\Gamma_{a,Y}]^{-1}_{j,j'}$ denotes the (j, j')-element of the inverse to the matrix

$$\Gamma_{a,Y}(z) = \left[\left(a_j - \tfrac{\mathrm{i}z}{4\pi}\right) \delta_{jj'} - \widetilde{G}_z(y_j - y_{j'}) \right]_{j,j'=1}^{N}, \quad \widetilde{G}_z(x) := \begin{cases} G_z(x), & x \neq 0, \\ 0, & x = 0. \end{cases} \quad (2.2)$$

The multi-set of (continuation) resonances $\Sigma(H)$ associated with the operator H (in short, resonances of H) is by definition the set of zeroes of the determinant $\det \Gamma_{a,Y}(\cdot)$, which we will call the characteristic determinant. This definition follows [15] and slightly differs from the one used in [5, 3] because isolated eigenvalues are now also included into $\Sigma(H)$. For the origin of this and related approaches to the understanding of resonances, we refer to [5, 15, 28, 29] and the literature therein. The multiplicity of a resonance k will be understood as the multiplicity of a corresponding zero of the analytic function $\det \Gamma_{a,Y}(\cdot)$ (see [3]).

An important common feature of quantum graphs and point interaction Hamiltonians is that the function that is used to determine resonances as its zeroes is an exponential polynomial. That is, the function

$$D(z) := (-4\pi)^N \det \Gamma_{a,Y}(z) \quad (2.3)$$

has the form

$$\sum_{j=0}^{\nu} P_{b_j}(z) e^{\mathrm{i}b_j z}, \quad (2.4)$$

where $\nu \in \mathbb{N} \cup \{0\}$, $b_j \in \mathbb{C}$, and $P_{b_j}(\cdot)$ are polynomials. One can see that, for the particular case of $D(\cdot)$, b_j are real and nonnegative numbers.

In what follows, we assume that the polynomials $P_{b_j}(\cdot)$ in the representation (2.4) for $D(\cdot)$ are nontrivial in the sense that $P_{b_j}(\cdot) \not\equiv 0$, and that all b_j in (2.4) are distinct and ordered such that

$$b_0 < b_1 < \cdots < b_\nu .$$

Under these assumptions, the set $\{b_j\}_{j=0}^{\nu}$ and the representation (2.4) are unique.

It is obvious that $b_0 = 0$ and the corresponding polynomial is equal to

$$P_0(z) = \prod_{j=1}^{N} (\mathrm{i}z - 4\pi a_j).$$

It is easy to notice [6] that $\nu \geq 1$, i.e., there are at least two summands in the sum (2.4) and at least one of them involves nonzero number b_j. (Let us recall that $N \geq 2$ is assumed throughout the paper.)

The asymptotic behavior of the counting function $\mathcal{N}_H$ for resonances of H is given by the formula

$$\mathcal{N}_H(R) = \frac{b_\nu}{\pi} R + O(1) \quad \text{as } R \to \infty, \tag{2.5}$$

which was derived in [25] from [12, Theorem 3.1] (for more general versions of this result in the context of the general theory of exponential polynomials see [9] and references therein). So, following the terminology of [25],

$$b_\nu \text{ is the effective size } W(H) \tag{2.6}$$

associated with the N-tuples Y and a that define the Hamiltonian H.

Remark 2.1. This raises the natural question of whether there exist a family of centers Y such that the effective size $W(H_{a,Y})$ of $H_{a,Y}$ might change with the change of the 'strength' tuple $a \in \mathbb{C}^N$. (Note that we do not allow a_j to take the value ∞. Otherwise, the answer becomes obvious since $a_j = \infty$ means that the center y_j is excluded from Y, see [3, 6]).

3. Absence of cancellations in Leibniz formula

In this section, we assume that the tuple a is fixed and consider the operator H and the set $\Sigma(H)$ of its resonances as functions of the family Y of interaction centers. Therefore we will use the notation H_Y for H, and

$$D_Y(z) := (-4\pi)^N \det \Gamma_{a,Y}(z) \tag{3.1}$$

for the corresponding modified version (2.3) of the characteristic determinant (2.2).

The Leibniz formula expands $D_Y(z)$ into the sum of terms

$$e^{\mathrm{i}zV_\sigma(Y)} P^{[\sigma,Y]}(z) \tag{3.2}$$

taken over all permutations σ in the symmetric group S_N, where the constants $V_\sigma(Y) \geq 0$ depends on σ and Y, and $P^{[\sigma,Y]}(\cdot)$ are polynomials in z depending on

σ and Y. They have the form

$$V_\sigma(Y) := \sum_{j=1}^{N} |y_j - y_{\sigma(j)}| = \sum_{j:\sigma(j)\neq j} |y_j - y_{\sigma(j)}|, \tag{3.3}$$

$$P^{[\sigma,Y]}(z) := (-1)^{\epsilon_\sigma} K_1(\sigma, Y) \prod_{j:\sigma(j)=j} (\mathrm{i}z - 4\pi a_j), \tag{3.4}$$

where K_1 is the positive constant depending on σ and Y,

$$K_1(\sigma, Y) := \prod_{j:\sigma(j)\neq j} |y_j - y_{\sigma(j)}|^{-1}$$

($K_1(\mathfrak{e}, Y) := 1$ in the case where σ is the identity permutation $\mathfrak{e} = [1][2]\dots[N]$) and ϵ_σ is the permutation sign (the Levi-Civita symbol).

Here and below we use the square brackets notation of the textbook [24] for permutation cycles, omitting sometimes, when it is convenient, the degenerate cycles consisting of one element. For each permutation σ, there exists a decomposition

$$\sigma = \prod_{m=1}^{M(\sigma)} \mathfrak{c}_m \tag{3.5}$$

of σ into disjoint cycles $\mathfrak{c}_m$ (in short, the *cycle decomposition* of σ). The changes in the order of cycles in the product (3.5) does not influence the result of the product. Up to such variations of order, the decomposition (3.5) is unique (see, e.g., [24]). So the number $M(\sigma)$ of cycles in (3.5) is a well defined function of σ. It is connected with the permutation sign ϵ_σ by the well-known equality

$$\epsilon_\sigma = (-1)^{N-M(\sigma)}. \tag{3.6}$$

(To see this it is enough to conclude from the equality $[1\ 2 \dots\ n] = [1\ 2][2\ 3]\dots[(n-1)\ n]$ that the sign of a cycle $\mathfrak{c}_m$ equals to $(-1)^{\#(\mathfrak{c}_m)-1}$, where $\#(\mathfrak{c}_m)$ is the number of elements involved in the cycle $\mathfrak{c}_m$.)

We will use some basic notions of graph theory that are concerned with the directed and undirected graphs with lengths. Such graphs can be realized as metric graphs or as weighted discrete graphs. Because of connections of the topic of this paper with quantum graphs (see [25]), we try to adapt terminology and notation close to (but not coinciding with) that of the monographs [8, 27].

The numbers $V_\sigma(Y)$ have a natural geometric description from the point of view of pseudo-orbits of directed metric graph having vertices at the centers y_j, $j = 1, \dots, N$ (see [25] and references therein). Namely, $V_\sigma(Y)$ is the *metric length* (the sum of length of bonds) of the *directed graph* $\overrightarrow{\mathcal{G}_\sigma}$ associated with $\sigma \in S_N$ and consisting, by definition, of *bonds* $y_j \rightsquigarrow y_{\sigma(j)}$, $j = 1, \dots, N$, of metric length $|y_j - y_{\sigma(j)}|$. Note that loops of zero length from a vertex to itself are allowed in $\overrightarrow{\mathcal{G}_\sigma}$. Namely, in the case where the cycle decomposition of a permutation σ includes a degenerate cycle $[j]$ (i.e., $j = \sigma(j)$), the bond $y_j \rightsquigarrow y_{\sigma(j)}$ degenerates into the loop $y_j \rightsquigarrow y_j$ from y_j to itself, which has zero length. If the cycle decomposition of σ contains the cycle $[j\ \sigma(j)]$, then the corresponding cycle of the directed graph $\overrightarrow{\mathcal{G}_\sigma}$ consists of the two bonds $y_j \rightsquigarrow y_{\sigma(j)}$, $y_{\sigma(j)} \rightsquigarrow y_j$ between j and $\sigma(j)$ with two opposite directions, and so, the contribution of this cycle to the metric length of $\overrightarrow{\mathcal{G}_\sigma}$ is $2|y_j - y_{\sigma(j)}|$.

This, in particular, explains why the number

$$V(Y) = \max_{\sigma \in S_N} V_\sigma(Y) \tag{3.7}$$

is called in [25] the size of Y.

The coefficients b_j in (2.4) are called *frequencies* of the corresponding exponential polynomial $D_Y(\cdot)$. Similarly, $V_\sigma(Y)$ is the frequency of the term (3.2) in the Leibniz formula. By (3.7), there exists a term of the form (3.2) that has $V(Y)$ as its frequency. In the process of summation of the terms (3.2) in the Leibniz formula some of the terms may cancel so that, for a certain permutation $\sigma \in S_N$, $V_\sigma(Y)$ is not a frequency of $D_Y(\cdot)$. If this is the case, we say that there is *frequency cancelation* for the frequency $V_\sigma(Y)$. An example of frequency cancelation for the highest possible frequency $V(Y)$ have been constructed in [25] to prove that non-Weyl asymptotics is possible for $H_{a,Y}$.

By $\mathcal{G}_\sigma$ we denote the metric pseudograph (i.e., the undirected metric graph with possible degenerate loops and multiple edges) that is produced from the directed graph $\overrightarrow{\mathcal{G}_\sigma}$ by stripping off the direction for all bonds. So if $\sigma(j) = j$, $\mathcal{G}_\sigma$ contains the loop-edge $y_j \sim y_j$ of zero length. If $\sigma(j) \neq j$ and $\sigma(\sigma(j)) = j$, $\mathcal{G}_\sigma$ contains two identical edges $y_j \sim y_{\sigma(j)}$ each of them contributing to the metrical length $V_\sigma(Y)$ of $\mathcal{G}_\sigma$ (that is the multiplicity of the edge $y_j \sim y_{\sigma(j)}$ is 2). These two cases describe all "nonstandard" situations where the multiplicity of an edge is strictly larger than 1, or a loop can appear in $\mathcal{G}_\sigma$. That is, if $\sigma(j) \neq j \neq \sigma(\sigma(j))$, then $\mathcal{G}_\sigma$ has exactly two edges involving y_j, namely, $y_j \sim y_{\sigma^{\pm 1}(j)}$, which are distinct and of multiplicity 1.

Definition 3.1. We will say that two permutations σ and σ' are *edge-equivalent* and write $\sigma \cong \sigma'$ if $\mathcal{G}_\sigma = \mathcal{G}_{\sigma'}$.

Here the equality $\mathcal{G}_\sigma = \mathcal{G}_{\sigma'}$ is understood in the following sense: for any $j, j' \in [1, N] \cap \mathbb{N}$,

$$\text{the multiplicities of the edge } y_j \sim y_{j'} \text{ in the graphs } \mathcal{G}_\sigma \text{ and } \mathcal{G}_{\sigma'} \text{ coincide.} \tag{3.8}$$

It is easy to see that $\sigma \cong \sigma'$ exactly when the cycle decomposition of σ' can be obtained from that of σ by inversion of some of the cycles, i.e., for σ with the cycle decomposition (3.5), the edge-equivalence class of σ consists of permutations of the form $\prod_{m=1}^{M(\sigma)} \mathfrak{c}_m^{\alpha_m}$, where each α_m takes either the value 1, or -1.

From (3.6) and (3.3) we see that,

$$\text{if } \sigma \cong \sigma', \text{ then } \epsilon_\sigma = \epsilon_{\sigma'} \text{ and } V_\sigma(Y) = V_{\sigma'}(Y). \tag{3.9}$$

The reason for the introduction of the edge-equivalence is the following statement.

Proposition 3.1. *Assume that Y is such that the following assumption holds:*

$$V_\sigma(Y) = V_{\sigma'}(Y) \text{ only if } \sigma \cong \sigma'. \tag{3.10}$$

Then the Weyl-type asymptotics takes place, i.e., $W(H_{a,Y}) = V(Y)$.

Proof. Under condition (3.10), it is clear from (3.9) and the form (3.4) of the polynomials $P^{[\sigma,Y]}(\cdot)$, that in the process of summation of (3.2) by the Leibniz formula the terms with the frequency $V(Y)$ cannot cancel each other in $D_Y(\cdot)$. Thus, $V(Y) = b_\nu = W(H_{a,Y})$ (see (2.5), (2.6)). □

Theorem 3.2. *Let $\sigma, \sigma' \in S_N$. Then the following statements are equivalent:*

(i) $\sigma \cong \sigma'$;
(ii) $V_\sigma(Y) = V_{\sigma'}(Y)$ *for all* $Y \in \mathbb{A}$;
(iii) $V_\sigma(Y) = V_{\sigma'}(Y)$ *for all Y in a certain open ball* $\mathbb{B}_{\delta_0}(Y_0)$ *of the metric space* $\mathbb{A}$, *where* $\delta_0 > 0$ *and* $Y_0 \in \mathbb{A}$.

3.1. Proof of Theorem 3.2

The implications (i) $\Longrightarrow$ (ii) $\Longrightarrow$ (iii) are obvious.
Let us now prove (iii) $\Longrightarrow$ (ii).

Lemma 3.3. *Let the closed segment* $[Y_0, Y_1] = \{Y(t) = (1-t)Y_0 + tY_1 \ : \ t \in [0,1]\}$ *belong to the set $\mathbb{A}$ and $Y_0 \neq Y_1$. Let Y_0 satisfy statement* (iii) *of Theorem* 3.2. *Then:*

(1) $V_\sigma(Y) = V_{\sigma'}(Y)$ *for all* $Y \in [Y_0, Y_1]$;
(2) Y_1 *satisfies statement* (iii) *of Theorem* 3.2 *in the sense that* $V_\sigma(Y) = V_{\sigma'}(Y)$ *for all* $Y \in \mathbb{B}_{\delta_1}(Y_1)$ *with a certain* $\delta_1 > 0$.
(3) *statement* (ii) *of Theorem* 3.2 *is satisfied, i.e.,* $V_\sigma(Y) = V_{\sigma'}(Y)$ *for all* $Y \in \mathbb{A}$.

Proof. Let $\delta_2 := \min\{|y - Y(t)|_2 \ : \ y \in \operatorname{bd}\mathbb{A}, \ t \in [0,1]\}$, where

$$\operatorname{bd}\mathbb{A} := \{y \in (\mathbb{R}^3)^N \ : \ y_j = y_{j'} \ \text{ for a certain } \ j \neq j'\}$$

is the boundary of the set $\mathbb{A}$ in the normed space $(\mathbb{R}^3)^N$. Since $[Y_0, Y_1] \subset \mathbb{A}$ and $\mathbb{A}$ is open in $(\mathbb{R}^3)^N$, we see that $\delta_2 > 0$.

(1) Consider the function $f(t) = V_\sigma(Y(t)) - V_{\sigma'}(Y(t))$ for $t \in (-\delta_3, 1+\delta_3)$, where $\delta_3 := \delta_2 / |Y_1 - Y_0|_2$.

It follows from (3.3) that $f(\cdot)$ is analytic in the interval $(-\delta_3, 1+\delta_3)$. Indeed, $|y_j - y_{j'}| = \left(\sum_{m=1}^3 (y_{j,m} - y_{j',m})^2\right)^{1/2}$, where $y_{j,m}$ and $y_{j',m}$, $m = 1,2,3$, are the $\mathbb{R}^3$-coordinates of y_j and $y_{j'}$, respectively. Since $Y(t) \in \mathbb{A}$ for this range of t, the sum cannot be 0 for $j \neq j'$, and we see that, for $(y_j(t))_{j=1}^N = Y(t)$, each $|y_j(t) - y_{j'}(t)|$ is a composition of functions which are analytic in t.

Hence, we can consider a complex t and extend $f(\cdot)$ as an analytic function in a neighborhood of $(-\delta_3, 1+\delta_3)$ in the complex plane $\mathbb{C}$. Since Y_0 satisfies (iii), we have $f(t) = 0$ in a neighborhood of 0. Due to analyticity, $f(t) = 0$ for all $t \in (-\delta_3, 1+\delta_3)$. This proves (1).

(2) It follows from the definition of δ_2 that $[Y_0, Y] \subset \mathbb{A}$ for every $Y \in \mathbb{B}_{\delta_2}(Y_1)$. So statement (1) of the lemma can be applied to each of these segments. This gives claim (2).

(3) follows from statement (2) and the fact that $\mathbb{A}$ is piecewise linear path connected in $(\mathbb{R}^3)^N$. □

Let us prove (ii) $\Longrightarrow$ (i). Assume that $\sigma \not\cong \sigma'$. Then, by Definition 3.1 and (3.8), there exists a center y_{j_*} such that the sets of centers which are connected with y_{j_*} in the graphs $\mathcal{G}_\sigma$ and $\mathcal{G}_{\sigma'}$ do not coincide. This can happen in several situations, which, by a possible exchange of roles between σ and σ', can be reduced to the following six cases:

(a) $\sigma(j_*) = j_*$ and $\sigma'(j_*) \neq j_*$.

(b) Both graphs $\mathcal{G}_\sigma$ and $\mathcal{G}_{\sigma'}$ have the common nondegenerate edge $y_{j_*} \sim y_{j_1}$ of multiplicity one, but the second edge involving y_{j_*} in $\mathcal{G}_\sigma$ and $\mathcal{G}_{\sigma'}$ do not coincide. To be specific let us assume that $\mathcal{G}_\sigma$ and $\mathcal{G}_{\sigma'}$ have the edges $y_{j_*} \sim y_j$ and $y_{j_*} \sim y_{j'}$, resp., and that y_{j_*}, y_{j_1}, y_j, $y_{j'}$ are distinct centers.

(c) The graph $\mathcal{G}_\sigma$ has two edges $y_{j_*} \sim y_{j_m}$, $m = 1, 2$, the graph $\mathcal{G}_{\sigma'}$ has two edges $y_{j_*} \sim y_{j'_m}$, $m = 1, 2$, and all the five centers y_{j_*}, y_{j_m}, $y_{j'_m}$, $m = 1, 2$, are distinct.

(d) The graph $\mathcal{G}_\sigma$ has the edge $y_{j_*} \sim y_j$ of multiplicity 2, the graph $\mathcal{G}_{\sigma'}$ has two edges $y_{j_*} \sim y_{j'_m}$, $m = 1, 2$, and the 4 centers y_{j_*}, y_j, $y_{j'_1}$, $y_{j'_2}$ are distinct.

(e) The graph $\mathcal{G}_\sigma$ has the edge $y_{j_*} \sim y_{j_1}$ of multiplicity 2, the graph $\mathcal{G}_{\sigma'}$ has two edges $y_{j_*} \sim y_{j_1}$, $y_{j_*} \sim y_{j_2}$, and the 3 centers y_{j_*}, y_{j_1}, y_{j_2} are distinct.

(f) The graph $\mathcal{G}_\sigma$ has the edge $y_{j_*} \sim y_j$ of multiplicity 2, the graph $\mathcal{G}_{\sigma'}$ has the edge $y_{j_*} \sim y_{j'}$ of multiplicity 2, and the 3 centers y_{j_*}, y_j, $y_{j'}$ are distinct.

Let us show that, for each of the 6 above situations, statement (ii) of Theorem 3.2 does not hold true under the assumption that $\sigma \not\cong \sigma'$.

Case (a). The function $V_\sigma(Y)$ is obviously constant for all small changes of y_{j_*} since this center is connected only with itself in $\mathcal{G}_\sigma$. This is not true for $V_{\sigma'}(Y)$ because in $\mathcal{G}_{\sigma'}$, y_{j_*} is connected with at least one of the other centers. Hence, statement (ii) of Theorem 3.2 does not hold true.

Case (b). Let us take for $t \in (0, 1)$, $Y(t) \in \mathbb{A}$ such that $y_{j_*} = (1-t)y_j + ty_{j'}$, but all the centers except y_{j_*} do not depend on t. Then as t changes in $(0, 1)$, the function $V_\sigma(Y(t)) - V_{\sigma'}(Y(t))$ is strictly increasing. This contradicts statement (ii) of Theorem 3.2.

Cases (c)–(f) can be treated by arguments similar to that of Case (b) with some modifications, which we consider briefly below.

Case (c). One can take $Y(t)$, $t \in (-1, 1)$, such that for $m = 1, 2$, the $\mathbb{R}^3$-coordinates of y_{j_m} are $(-m, 0, 0)$, the $\mathbb{R}^3$-coordinates of $y_{j'_m}$ are $(m, 0, 0)$, and put $y_{j_*} = (t, 0, 0)$. Thus, $V_\sigma(Y(t)) - V_{\sigma'}(Y(t))$ is strictly increasing for $t \in (-1, 1)$ and so the statement (ii) of Theorem 3.2 does not hold.

Case (d). In the graph $\mathcal{G}_\sigma$, the center y_{j_*} is connected only with y_j. That is why it is easy to construct the evolution $Y(t)$ of Y in such a way that only y_{j_*} moves, the distance $|y_{j_*} - y_j|$ is constant, but $\sum_{m=1,2} |y_{j_*} - y_{j'_m}|$ changes, and so also $V_{\sigma'}(Y(t))$ changes contradicting the statement (ii) of Theorem 3.2. For example, let $y_{j'_m} = ((-1)^m, 0, 0)$ for $m = 1, 2$, $y_j = (0, 1, 0)$, and assume that $y_{j_*}(t)$ move along a circle of radius 1 in Ox^1x^2-plane.

Case (e). It is enough to choose $y_{j_*}(t) = (1-t)y_{j_1} + ty_{j_2}$ for $t \in (0,1)$ with all other centers fixed, and then to follow arguments of Case (b).

Case (f). It is enough to put $y_{j_*}(t) = (1-t)y_j + ty_{j'}$ and use the arguments of Case (b). This completes the proof of Theorem 3.2.

3.2. Proof of Theorem 1.1

Let us denote by $n \in \mathbb{N}$ the number of edge-equivalence classes in S_N and let us take one representative $\widetilde{\sigma}_j$, $j = 1, \dots, n$, in each of them. Let

$$\mathbb{A}_1 := \{Y \in \mathbb{A} \ : \ V_{\widetilde{\sigma}_j}(Y) \neq V_{\widetilde{\sigma}_m}(Y) \text{ if } j \neq m\}.$$

Lemma 3.4. *The set $\mathbb{A}_1$ is open and dense in the metric space $\mathbb{A}$.*

Proof. Consider the sets

$$\mathbb{A}^{j,m} := \{Y \in \mathbb{A} \ : \ V_{\widetilde{\sigma}_j}(Y) \neq V_{\widetilde{\sigma}_m}(Y)\}, \quad j, m = 1, \dots, n.$$

Since the functions $V_{\widetilde{\sigma}_j}(\cdot)$ are continuous in $\mathbb{A}$, the sets $\mathbb{A}^{j,m}$ are open.

Let us show that $\mathbb{A}^{j,m}$ is dense in $\mathbb{A}$ whenever $j \neq m$. Assume ad absurdum that the converse is true. Then statement (iii) of Theorem 3.2 holds for $\widetilde{\sigma}_j$ and $\widetilde{\sigma}_m$. By Theorem 3.2, $\widetilde{\sigma}_j \cong \widetilde{\sigma}_m$. This contradicts the choice of $\widetilde{\sigma}_j$ and $\widetilde{\sigma}_m$ as representative of different edge-equivalence classes.

We see that $\mathbb{A}_1 = \bigcap_{1 \leq j < m \leq n} \mathbb{A}^{j,m}$ is the intersection of a finite number of open dense sets. This completes the proof. $\square$

Proposition 3.1 shows that for each $Y \in \mathbb{A}_1$ and each $a \in \mathbb{C}^N$ the Weyl-type asymptotics of $\mathcal{N}_{H_{a,Y}}(\cdot)$ takes place. This completes the proof of Theorem 1.1.

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Spectral clusters, asymmetric spaces, and boundary control for Schrödinger equation with strong singularities

Sergei Avdonin and Julian Edward

Abstract. We consider a linear system composed of $N+1$ Schrödinger equations connected by point-mass-like interface conditions. We show that the system is exactly controllable with a Dirichlet boundary control at one end, and various homogeneous boundary conditions on the other end. The reachable set is characterized by spectral data. We then study the regularity of the reachable functions using a family of Riesz bases of asymmetric spaces.

Devoted to memory of Boris Sergeevich Pavlov, outstanding mathematician and great person, who was a teacher of many St. Petersburg mathematicians including the first author of this paper.

1. Introduction

Asymmetric spaces arise naturally in evolution equations with strong singularities. The first time this was studied in the context of control theory was, to the best our knowledge, in [21], which considered a vibrating string with one attached mass, also see [12, 13, 4, 5]. Asymmetric spaces associated to point masses have also been observed for a Rayleigh beam [14], but not for Euler–Bernoulli beams, see [26, 15]. Internal point masses have also been considered for the heat equation [20].

In this current work, we study controllability results for the following system based on the Schrödinger wave equation, featuring point-mass-like interface

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conditions:

$$
\begin{aligned}
i\frac{\partial u}{\partial t}-\frac{\partial^2 u}{\partial x^2}+qu=0, &\quad t\in(-\infty,T),\ x\in(0,l)\setminus\{a_j\}_{j=1}^N, \qquad (1.1)\\
u(x,t)=0, &\quad t\le 0,\\
u(0,t)=f(t),&\\
\beta_1 u(l,t)+\beta_2 u_x(l,t)=0,&\\
u(a_j^-,t)=u(a_j^+,t)=u(a_j,t), &\quad j=1,\dots,N,\\
u_x(a_j^+,t)-u_x(a_j^-,t)=iM_j u_t(a_j,t). & \qquad (1.2)
\end{aligned}
$$

In what follows, we will refer to $\beta_2=0$ as Dirichlet boundary conditions at $x=l$, and all other cases as "mixed" boundary conditions. We will assume throughout that $f\in L^2(0,T)$ for some $T>0$, and that $(\beta_1,\beta_2)\neq(0,0)$. In what follows, we will refer to the singularities at $x=a_j$ as "masses". Let q_j be the restrictions of q to the interval (a_j,a_{j+1}). Following [4], we assume throughout that for $j=0,1,2$, that q_j extends to $C[a_j,a_{j+1}]$, while for $j>2$, q_j extends to a function in $C^{j-2}[a_j,a_{j+1}]$.

To state the results, we first discuss the underlying Sturm–Liouville problem. Let $A^{\mathcal{D}}$, resp. $A^{\mathcal{M}}$, be the semi-bounded, self-adjoint operator for the associated Sturm–Liouville problem on an appropriately defined Hilbert space L^2_M and with the Dirichlet, resp. mixed, boundary condition at $x=l$. Fix b equal either $\mathcal{D}$ or $\mathcal{M}$. We use A^b to construct Sobolev-type spaces $\mathcal{H}^{s,b}$. Then we have:

Proposition 1. *Assume $b=\mathcal{D}$ or $\mathcal{M}$. Suppose u solves the system* (1.1)–(1.2)*. Then the mapping $t\mapsto u^f(x,t)$ is a continuous mapping $\mathbb{R}\mapsto\mathcal{H}^{-1,b}(0,l)$.*

This result is proven in Sect. 3. In Sect. 2, it is shown that $\mathcal{H}^{-1,\mathcal{D}}=H^{-1}(0,l)$

In the case of no masses ($M_j=0$) and Dirichlet boundary condition at $x=l$, it was proven in [25] that for any $T>0$, the reachable set is $H^{-1}(0,l)$; more precisely, for any $v\in H^{-1}(0,l)$ and any $T>0$, there exists $f\in L^2(0,T)$ such that $u(\cdot,T)=v(\cdot)$ as elements of H^{-1}. In the case of one positive mass, the system was studied recently by Hansen in [19]. In that work, the author assumed also $a_1=l/2$, and $q=0$ and assumed Dirichlet boundary condition at $x=l$. He proved that for any $T>0$, the reachable set was the $H^{-1}(0,l)$; thus reachable set is symmetric in the sense that its elements are H^{-1} both to the left and to the right of $x=l/2$. The author then considered Neumann control at $x=0$ with Dirichlet boundary condition at $x=l$. Somewhat surprisingly, for any $T>0$, the reachable set in this case is asymmetric in the sense that it is $L^2(0,l/2)$ to the left of the mass, and $H^1(l/2,l)$ to the right. The result for Dirichlet control shows that the presence of the mass does not itself cause the asymmetry of the reachable set.

One result in this paper is that for the Dirichlet boundary condition, the reachable set is not always $H^{-1}(0,l)$.

Theorem 1. *Suppose $M=N=1$, $l=1$, and $q=0$, and assume Dirichlet boundary condition at $x=1$. Then the reachable set is $H^{-1}(0,1)$ if and only if $a_1\in\{p/(p+1):\ p\in\mathbb{N}\}$.*

The proof of this result, and also Hansen's, uses a rather precise analysis of the spectral asymptotics of the associated Sturm–Liouville problem. The key element of the proof is either the existence or the non-existence of a certain subsequence of eigenvalues which are uniformly separated from the rest of the spectrum. Without such a sequence, the reachable set is $H^{-1}(0,1)$. It appears difficult to extend these methods to the most general case in the system (1.1)–(1.2).

To further study the general case using spectral methods, we apply the theory of Riesz bases of exponential functions as developed by Pavlov [27] and use the results in this area obtained in [2, 3, 7, 8]. To give a spectral characterization of the reachable set, in Sect. 4.2 we will parametrize the spectrum of A^b as

$$\{\mu_j^p \ : \ p \in \mathbb{N}, \ j = 1, \ldots, \mathcal{N}^{(p)}\}$$

where $\mathcal{N}^{(p)} \le N + 1$. This parametrization is designed so that for each p the set $\left\{\sqrt{\mu_1^p}, \ldots, \sqrt{\mu_{\mathcal{N}^{(p)}}^p}\right\}$ are close together. Let φ_j^p be a unit norm eigenfunction associated to μ_j^p. Defining

$$\zeta(p,k) = \sum_{j=k}^{\mathcal{N}^{(p)}} \varphi_j^p(x)(\varphi_j^p)'(0) \prod_{l=1}^{k-1} \left(\mu_j^p - \mu_l^p\right),$$

we use exponential divided differences to prove that the reachable set, denoted R^b, is given by

$$R^b = \left\{ \sum_{p=1}^{\infty} \sum_{k=1}^{\mathcal{N}^{(p)}} c_{p,k}\zeta(p,k), \text{ with } c_{p,k} \in \ell^2 \right\}.$$

More precisely,

Theorem 2. *Fix $b = \mathcal{M}$ or $\mathcal{D}$. Let $v \in R^b$. Then for any $T > 0$, there exists $f \in L^2(0,T)$ such that u solving the system* (1.1)–(1.2) *satisfies $u(x,T) = v(x)$ as elements of $\mathcal{H}^{-1,b}$.*

The proof of this result, and also of some estimates on $||f||_{L^2(0,T)}$, will be given in Sect. 5.

The main focus of this work will be study the local regularity of functions in R^b. To this end, we will apply to this problem the framework developed in [4] and [5]. In these works, we studied the exact boundary controllability for a vibrating string with N attached masses. Let $w(x,t)$ solve

$$\begin{aligned}\frac{\partial^2 w}{\partial t^2} - \frac{\partial^2 w}{\partial x^2} + q(x)w = 0, \quad t \in (0,T),\ x \in (0,l) \setminus \{a_j\}_{j=1}^N,\\ w(x,t) = 0, \quad t \le 0,\\ w(a_j^-,t) = w(a_j^+,t) = w(a_j,t), \quad j = 1,\dots,N,\\ M_j w_{tt}(a_j,t) = w_x(a_j^+,t) - w_x(a_j^-,t),\\ w(0,t) = f(t),\\ \beta_1 w(l,t) + \beta_2 w_x(l,t) = 0. \end{aligned} \tag{1.3}$$

This system is well posed in asymmetric spaces whose regularity to the right of each mass exceeds the regularity to the left by one Sobolev order. More precisely, for $f \in L^2$, we have $(w, w_t) \in W_0^b \times W_{-1}^b$, where W_i^b are subsets of $\oplus_{j=0}^N H^{i+j}(a_j, a_{j+1}) \oplus (\mathbb{R}^N)$. Here the elements of $\mathbb{R}^N$ will account for the position of the masses. The formal definition of W_i^b, which is somewhat technical, is deferred until Sect. 4. One of the main results in [4] and [5] was to construct Riesz bases of $W_i^{\mathcal{D}}$ in terms of $\{\mu_j^p, \varphi_j^p\}$. This construction will also give similar Riesz bases for $W_i^{\mathcal{M}}$. By comparing the terms in these Riesz bases with $\zeta(p,k)$, we prove

Theorem 3. *Fix $b = \mathcal{M}$ or $\mathcal{D}$. The following inclusions are valid:*

$$W_{-1}^b \subset R^b \subset \mathcal{H}^{-1,b}(0,l).$$

Furthermore, let

$$v = \sum_{p=1}^{\infty} \sum_{k=1}^{\mathcal{N}^p} c_{p,k} \zeta(p,k) \in R^b.$$

Then there exist positive constants C_1, C_2 such that

$$C_1 ||v||^2_{W^b_{-N-1}} \le \sum_{p=1}^{\infty} \sum_{k=1}^{\mathcal{N}^p} |c_{p,k}|^2, \tag{1.4}$$

and if $v \in W_{-1}^b$, then

$$\sum_{p=1}^{\infty} \sum_{k=1}^{\mathcal{N}^p} |c_{p,k}|^2 \le C_2 ||v||^2_{W^b_{-1}}. \tag{1.5}$$

Of course, $||v||^2_{W^b_{-1}}$ is possibly infinite, in which case the second inequality will be vacuous.

One can refine Theorem 3 if the clusters have small cardinality.

Proposition 2. *Let $J \in \{1,\dots,N+1\}$. The condition*

$$\#\{p :\ \mathcal{N}^p \ge J\} = \infty, \tag{1.6}$$

is necessary and sufficient for there to exist

$$v \in R^b \cap \left(W^b_{-J} \setminus W^b_{-J+1}\right).$$

The following corollaries will now follow easily for mixed boundary conditions at $x = l$.

Corollary 1. *Let* $l_j = a_{j+1} - a_j$*. Assume*

$$\frac{l_j}{l_N} \in \mathbb{Q} \quad \textit{and} \quad \frac{l_j}{l_N} \neq \frac{2m}{2n+1}, \qquad \forall m, n \in \mathbb{N},\ j = 0, \dots, N-1.$$

Then $R^{\mathcal{M}} \subset W^{\mathcal{M}}_{-N}$*. In particular, the restriction to* (a_N, l) *of any reachable elements will be in* L^2*.*

Specializing to $N = 1$, we have a sharp characterization of the reachable set.

Corollary 2. *If* $N = 1$*, then* $R^{\mathcal{M}} = W^{\mathcal{M}}_{-1}$*.*

With Dirichlet boundary condition at $x = l$, however, (1.6) always holds with $J = N + 1$:

Proposition 3. *Assume Dirichlet boundary conditions at* $x = l$*. Then*

$$\#\big\{p :\ \mathcal{N}^p = N + 1\big\} = \infty. \tag{1.7}$$

The proof of this result uses a diophantine approximation argument.

We conclude this section by mentioning that the methods of this paper should also be adaptable to Neumann control. Also, in future work we plan to apply the analysis here to study the exact controllability of a certain system of beams with masses at their point of coupling.

The rest of the paper is organized as follows. The operator A^b and spaces $\mathcal{H}^{s,b}$, W^b_i will be defined in Sect. 2. In Sect. 3, we present the control problem as a moment problem, and we prove that the reachable set is always in $\mathcal{H}^{-1,b}$. We also prove Theorem 1. In Sect. 4 we define the exponential divided differences (EDD) and prove Proposition 3. In Sect. 5, we prove Theorems 2 and 3, Proposition 2, and Corollaries 1 and 2.

2. Preliminaries

2.1. Sturm–Liouville problem

The Sturm–Liouville problem associated to the system (1.1) is:

$$\begin{aligned} -\phi''(x) + q(x)\phi(x) &= \mu\phi(x), \quad x \in (0, l) \setminus \{a_j\}_1^N, \\ \beta_1\phi(l) + \beta_2\phi'(l) &= 0, \\ \phi(0) &= 0, \\ \phi(a_j^-) &= \phi(a_j) = \phi(a_j^+), \\ \phi'(a_j^+) &= \phi'(a_j^-) - M_j\mu\phi(a_j), \quad j = 1, \dots, N. \end{aligned} \tag{2.8}$$

We now discuss the self-adjoint operators associated to (2.8). In what follows, it will be convenient to define

$$L := -\frac{d^2}{dx^2} + q(x),$$

the differential operator acting on distributions living on $(0, a_1) \cup \cdots \cup (a_N, l)$. We define an associated Hilbert space L^2_M which accounts for ϕ's value at the masses. In particular, $(\phi(x), \phi(a_1), \ldots, \phi(a_N)) \in L^2_M$ if

$$||\phi||^2_M := \sum_{j=0}^{N} \int_{a_j}^{a_{j+1}} |\phi(x)|^2 dx \ + \sum_{j=1}^{N} M_j |\phi(a_j)|^2 < \infty.$$

Denote by $\langle \cdot, \cdot \rangle_M$ the associated inner product. This space is canonically isomorphic to $L^2(0, l) \oplus \mathbb{R}^N$. Here and it what follows $H^s(a_j, a_{j+1})$ refers to the standard Sobolev space, with $H^0 = L^2$.

We define a quadratic form on L^2_M by

$$Q^{\mathcal{D}}(u, v) = \sum_{j=0}^{N} \int_{a_j}^{a_{j+1}} (u'v' + quv)\, d\tau,$$

with domain

$$\mathcal{Q}^{\mathcal{D}} = \{u \in L^2_M(0, l) : u|_{(a_j, a_{j+1})} \in H^1(a_j, a_{j+1}),\ u(a_j^-) = u(a_j) = u(a_j^+), \\ j = 1, \ldots, N,\ \text{and } u(0^+) = u(l^-) = 0\}.$$

We also define, if $\beta_2 \neq 0$, a quadratic form by

$$Q^{\mathcal{M}}(u, v) = \sum_{j=0}^{N} \int_{a_j}^{a_{j+1}} (u'v' + quv)\, dx + \frac{\beta_1}{\beta_2} u(l)v(l),$$

with domain

$$\mathcal{Q}^{\mathcal{M}} = \{u \in L^2_M(0, l) : u|_{(a_j, a_{j+1})} \in H^1(a_j, a_{j+1}),\ u(a_j^-) = u(a_j) = u(a_j^+), \\ j = 1, \ldots, N,\ \text{and } u(0^+) = 0\}.$$

We remark in passing that the masses do not come into the definition of the quadratic forms. Associated with these semi-bounded, closed quadratic forms (and the norm $||u||_M$) are the self-adjoint operators A^b, with $b = \mathcal{D}$ or $\mathcal{M}$, and with operator domain

$$Dom(A^b) = \{u \in \mathcal{Q}^b :\ A^b(u) \in L^2_M(0, l)\}.$$

Then for $u \in Dom(A^b)$,

$$A^b u(x) = \begin{cases} (Lu)(x), & x \neq a_j,\ j = 1, \ldots, N, \\ \frac{1}{M_j}(u'(a_j^-) - u'(a_j^+)), & x = a_j,\ j = 1, \ldots, N. \end{cases} \tag{2.9}$$

Example 1. Set $q = 0$, $N = M = 1$, $l = 2$ and $a_1 = 1$. Let

$$u(x) = \begin{cases} 1 - |x - 1|, & x \neq 1, \\ 1, & x = 1, \end{cases}$$

so $u \in \mathcal{Q}^{\mathcal{D}}$. Then

$$A^D u(x) = \begin{cases} 0, & x \neq 1, \\ 2, & x = 1. \end{cases}$$

One can use standard spectral theory arguments to show that the spectrum of A^b is discrete. Let $\{(\lambda_n)^2\}_{n=1}^\infty$ be the set of eigenvalues of system (2.8) listed in increasing order. It follows by standard arguments that the eigenvalues are simple, see [4]. Let $\{\varphi_n\}$ be a basis of normalized eigenfunctions. By simplicity of the spectrum and the self-adjointness of A^b we have that the eigenfunctions are orthonormal with respect to $\langle\cdot,\cdot\rangle_M$.

We use the spectral representation to create a scale of Sobolev-type spaces.

Definition 1. *Let $b = \mathcal{D}$ or $\mathcal{M}$. Choose $E \geq 0$ such that $\mu_1 + E > 0$. Define*

$$\mathcal{H}^{s,b} = \left\{ u(x) = \sum_{n=1}^{\infty} a_n \phi_n(x) \ : \ ||u||_s^2 = \sum_{n=1}^{\infty} |a_n|^2 (\mu_n + E)^{s/2} < \infty \right\}, \quad s \in \mathbb{R}.$$

Thus $\mathcal{H}^{s,b} = Dom((A^b + E)^{s/2})$.

Associated to these spaces are various equations that hold at $x = a_j$. For instance, for $v \in \mathcal{H}^{s,b}$, $s \geq 1$, we have

$$v(a_j^-) = v(a_j) = v(a_j^+), \quad j = 1, \dots, N, \tag{2.10}$$

and for $v \in \mathcal{H}^{s,b}$ with $s \geq 3$, we have for $j = 1, \dots, N$,

$$\frac{1}{M_j}\big(v'(a_j^-) - v'(a_j^+)\big) = Lv(a_j^-) = Lv(a_j^+), \tag{2.11}$$

as well as (2.10). Clearly, these equations hold for v an eigenfunction, and so by basic Fourier theory they hold for all $v \in \mathcal{H}^{s,b}$. In what follows, we will refer to such equations as "compatibility conditions". We have the following list of all compatibility conditions.

Lemma 1. *For $s \geq 0$ and $v \in \mathcal{H}^{s,b}$, the following compatibility conditions hold for $j = 1, \dots, N$:*

$$v(a_j^-) = v(a_j) = v(a_j^+) \ \text{ for } s \geq 1, \quad \text{and} \ \ L^n v(a_j^-) = L^n v(a_j^+), \ 0 \leq n \leq \lceil s/2 \rceil - 1, \tag{2.12}$$

and for $0 \leq n \leq \lceil s/2 \rceil - 2$,

$$\frac{1}{M_j}\Big(\frac{d}{dx}(L^n v)(a_j^-) - \frac{d}{dx}(L^n v)(a_j^+)\Big) = L^{n+1}v(a_j^+) = L^{n+1}v(a_j^-). \tag{2.13}$$

Also, for $b = D$ we have

$$L^n v(0) = L^n v(l) = 0, \quad 0 \leq n \leq \lceil s/2 \rceil - 1, \tag{2.14}$$

while for $b = m$

$$L^n v(l) = 0, \ 0 \leq n \leq \lceil s/2 \rceil - 1, \quad (\beta_1 L^n v + \beta_2 L^n v')(l) = 0, \ 0 \leq n \leq \lfloor s/2 \rfloor - 1. \tag{2.15}$$

For proof of this result, the reader is referred to [4].

Remark 1. In (2.12), we interpret the condition $0 \leq n \leq -1$, which holds for $s = 0$, to mean no such compatibility condition holds.

Remark 2. Recall the well known Sobolev space

$$H_0^1(0,l) = \{u \in H^1(0,l) : u(0) = u(l) = 0\},$$

and its dual $H^{-1}(0,l)$. Then the following spaces are canonically isomorphic:

$$H_0^1(0,l) = \mathcal{H}^{1,\mathcal{D}} = \mathcal{Q}^{\mathcal{D}}.$$

Consequently, we can identify $\mathcal{H}^{-1,\mathcal{D}}(0,l) = H^{-1}(0,l)$.

2.2. Asymmetric spaces associated to wave equation

We discuss some asymmetric spaces that arise naturally in considering the regularity of the following wave equation. Suppose $u = (u(x,t), u(a_1,t), \dots, u(a_N,t))$ solves

$$\begin{aligned} \frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} + q(x)u = 0,\ t \in (0,T), \quad x \in (0,l) \setminus \{a_j\}_{j=1}^N, \\ u(x,t) = 0,\ t \leq 0, \\ u(a_j^-,t) = u(a_j,t) = u(a_j^+,t), \quad j = 1,\dots,N, \\ M_j u_{tt}(a_j,t) = u_x(a_j^+,t) - u_x(a_j^-,t), \quad j = 1,\dots,N, \\ u(0,t) = f(t), \\ \beta_1 u(l,t) + \beta_2 u_x(l,t) = 0. \end{aligned} \tag{2.16}$$

An important property of this system is that for the wave generated by f, as it propagates from left to right, the part of the wave that is transmitted across a mass will be one Sobolev order more regular than incoming wave, whereas the reflected part of the wave has the same Sobolev order as the incoming wave. This was first observed, to the best of our knowledge, in [21]. Below, we will define spaces that characterize the reachable set of positions and velocities for system (2.16), as was shown in [4].

Letting X' denote the dual space to X, define

$$\Theta^{-1}(0,a_1) := \{u \in H^1(0,a_1) : u(0) = 0\}'.$$

We define a scale of spaces by

$$W_i = \left((\oplus_{j=0}^N H^{i+j}(a_j,a_{j+1}))\right) \oplus \mathbb{R}^N \quad \text{for } i = 0,1,2,\dots,$$

and

$$W_{-1} = \Theta^{-1}(0,a_1) \oplus \left(\oplus_{j=1}^N H^{j-1}(a_j,a_{j+1})\right) \oplus \mathbb{R}^{N-1}.$$

Following [4], we pose certain compatibility conditions that solution u must satisfy at $\{a_j\}$. These conditions arise naturally from the equations in (2.16) provided u is sufficiently regular. These conditions resemble those listed for $\mathcal{H}^{s,b}$ in the previous subsection, but also account for the fact that a solution u to system (2.16) is more regular near $x = a_{j+1}$ than near $x = a_j$.

Definition 2. *Let $j = 1, \dots, N$, and let k be any integer. A function $\phi(x)$ satisfies Condition $\mathcal{C}^{k,\mathcal{D}}$ at $x = a_j$ if*

$$\frac{d}{dx}L^n\phi(a_j^-) = \frac{d}{dx}L^n\phi(a_j^+) - M_jL^{n+1}\phi(a_j^+) \tag{2.17}$$

is satisfied for $0 \le n \le \lceil k/2 \rceil - 2$, and

$$\phi(a_j) = \phi(a_j^+) \text{ if } k \ge 0, \text{ and } L^n\phi(a_j^-) = L^n\phi(a_j^+) \tag{2.18}$$

is satisfied for $0 \le n \le \lceil k/2 \rceil - 1$. For $j = 0$ or $(N+1)$, a function $\phi(x)$ satisfies Condition $\mathcal{C}^{k,\mathcal{D}}$ at $x = a_j$ if

$$L^n\phi(a_j) = 0, \; n = 0, 1, 2, \dots, \tag{2.19}$$

is satisfied for $0 \le n \le \lceil k/2 \rceil - 1$.

For convenience, for $k \le 0$ we denote Condition $\mathcal{C}^{k,\mathcal{D}}$ at $x = a_j$ to be a vacuous condition.

Definition 3. *A function satisfies Condition $\mathcal{C}_*^{i,\mathcal{D}}$ if it satisfies Condition $\mathcal{C}^{j-1+i,\mathcal{D}}$ at $x = a_j$ for all $j = 1, \dots, N+1$, and Condition $\mathcal{C}^{i,\mathcal{D}}$ at $x = 0$.*

A function satisfies Condition $\mathcal{C}_*^{i,\mathcal{M}}$ if it satisfies Condition $\mathcal{C}^{j-1+i,\mathcal{D}}$ at $x = a_j$ for all $j = 1, \dots, N$, Condition $\mathcal{C}^{i,\mathcal{D}}$ at $x = 0$, and

$$\beta_1(L^n\phi)(l) + \beta_2(L^n\phi_x)(l) = 0, \quad n \le \left\lfloor \frac{N-2+i}{2} \right\rfloor.$$

Definition 4. *Let $b = \mathcal{D}$ or $\mathcal{M}$. For integer $i \ge -1$, define the space*

$$W_i^b := \left\{\phi \in W_i : \; \phi \text{ satisfies Condition } \mathcal{C}_*^{i,b}\right\}.$$

Then W_i^b are real Hilbert spaces with inner product

$$\langle \phi, \psi \rangle_i = \sum_{j=0}^{N} \langle \phi, \psi \rangle_{H^{i+j}(a_j, a_{j+1})} + \sum_{j=1}^{N} M_j\phi(a_j^+)\psi(a_j^+). \tag{2.20}$$

Here we define

$$||\phi||^2_{H^n(a_j,a_{j+1})} = \left\|\frac{d^n\phi}{dx^n}\right\|^2_{L^2(a_j,a_{j+1})} + ||\phi||^2_{L^2(a_j,a_{j+1})}.$$

It is easy to see that we have a canonical inclusion of

$$W_i^b \subset \mathcal{H}^{i,b}.$$

Furthermore, the set of restrictions of elements of W_i^b to the interval (a_j, a_{j+1}) will be the same as the set of restrictions of elements of $\mathcal{H}^{i+j,b}$ to the same interval.

The following was proven in [5] for Dirichlet boundary conditions, and a similar proof works for mixed boundary condition at $x = l$.

Theorem 4. *Let $b = \mathcal{D}$ or $\mathcal{M}$. Choose a constant E so that $(A^b + E) > 0$. Let $i = 1, 2, \dots$ Then $(A^b + E)$ maps W_i^b bijectively onto W_{i-2}^b, and this mapping is an isomorphism with respect to the norms $|| \cdot ||_{W_i^b}$ and $|| \cdot ||_{W_{i-2}^b}$.*

Definition 5. *Choose E so that $(A^b + E) > 0$. For negative integer i, suppose $i+2n \geq 0$. Then we define $W_i^b = (A^b+E)^n(W_{i+2n}^b)$, with norm given by $||v||_{W_i^b} = ||\big(A^b + E\big)^{i/2}v||_{W_0^b}$ for i even, and $||v||_{W_i^b} = ||\big(A^b + E\big)^{(i+1)/2}v||_{W_{-1}^b}$ for i odd.*

The following relation now easily follows for any pair of integers j, k:

$$W_j^b \subset W_k^b \ \text{ if } j > k.$$

3. Spectral solution for the Schrödinger equation

3.1. An associated moment problem

In the first subsection here, we present the control problem as a moment problem. We use this to prove that the reachable set lies in $H^{-1}(0, l)$. In the second subsection, we consider the special case where $N = 1$ and $q = 0$, with Dirichlet boundary condition at $x = l$. In this case, precise spectral asymptotics are computed, and we are able to characterize the set of a_1 for which the reachable set equals $H^{-1}(0, l)$.

It will be useful to present the asymptotics of the eigenvalues $\{\mu_n : \ n \in \mathbb{N}\}$ for the system (2.8). Let

$$\lambda_n = \sqrt{\mu_n}.$$

Here we choose the square root of a negative real to have positive imaginary part. We will refer to the set $\Lambda := \{\lambda_n,\ n \in \mathbb{N}\}$ as the eigenfrequencies. Let $l_j = a_{j+1} - a_j$. The following result was proven in [5].

Theorem 5. (A) *Assume Dirichlet boundary conditions at $x = l$. Let Λ' be any subset of Λ obtained by deleting N elements. Then Λ' can be reparametrized as*

$$\Lambda' = \bigcup_{m=0}^{N} \{\lambda_m^{(k)}\}_{k\in\mathbb{K}},$$

where for each m,

$$\left|\lambda_m^{(k)} - \frac{\pi k}{l_m}\right| = O\big(|k|^{-1}\big).$$

(B) *Assume mixed boundary conditions at $x = l$. Let Λ' be any subset of Λ obtained by deleting N elements. Then Λ' can be reparametrized as*

$$\Lambda' = \left(\bigcup_{m=0}^{N-1} \{\lambda_m^{(k)}\}_{k\in\mathbb{K}}\right) \cup \{\lambda_N^{(k)}\}_{k\in\mathbb{Z}},$$

where for each $j < N$,

$$\left|\lambda_m^{(k)} - \frac{\pi k}{l_m}\right| = O\big(|k|^{-1}\big),$$

and

$$\left|\lambda_N^{(k)} - \frac{(2k+1)}{2}\frac{\pi}{l_N}\right| = O\big((|k|+1)^{-1}\big). \tag{3.21}$$

For the rest of this subsection, we will parametrize the frequencies by $\{\lambda_n\}$. In what follows, we denote by φ_n a unit-norm eigenfunction corresponding to λ_n.

We present the solution, u^f, of system (1.1) in the form of the series

$$u^f(x,t) = \sum_{n\in\mathbb{N}} a_n(t)\, \varphi_n(x). \tag{3.22}$$

We wish to find f solving

$$u^f(x,T) = v(x). \tag{3.23}$$

For any $f \in L^2(0,T)$, multiplying the equation (1.1) by $e^{it\mu_n}\varphi_n(x)$ and then integrating by parts gives for each n

$$a_n(t) = -i(\varphi_n)'(0) \int_0^t f(\tau) e^{i(t-\tau)\mu_n}\, d\tau. \tag{3.24}$$

We say that $\{a_n\} \in \ell^2_s$ if $\sum_1^\infty |a_n|^2 n^s < \infty$.

Proof of Proposition 1: It follows by [28, Chap. 1, Theorem 3] that

$$|(\varphi_n)'(0)| = O(n). \tag{3.25}$$

Also, by Theorem 5, either case A or B, the set $\{e^{it\mu_n} : n \in \mathbb{N}\}$ is a finite union of Riesz sequences in $L^2(0,T)$. It follows from (3.24) that $\{a_n(T)\} \in \ell^2_{-1}$, so by definition we have $u(x,T) \in \mathcal{H}^{-1,b}$. The proof of continuity follows from (3.24); the details are left to the reader.

We now formulate the control problem as a moment problem. Denote $e_n(t) = \exp(i\mu_n t)$. We set

$$\alpha_n = \frac{ia_n(T)}{(\varphi_n)'(0)}. \tag{3.26}$$

Let $\langle\cdot,\cdot\rangle_T$ be the standard complex inner product on $L^2(0,T)$. Let $f^T(t) = f(T-t)$. Then by (3.24), the control problem for $t = T$ can be written as

$$\alpha_n = \left\langle e_n, \overline{f}^T \right\rangle_T, \quad n \in \mathbb{N}. \tag{3.27}$$

There are two important points to be made about this moment problem. First, it is not certain in the general case that there exists a spectral gap, i.e., that

$$\inf_{m\neq n} |\mu_m - \mu_n| > 0.$$

As a consequence, it is not obvious that that $\{e_n\}$ forms a Riesz sequence. For this reason, in later sections we will rewrite this problem using Exponential Divided Differences. Second, an important role will be played by the asymptotics of $\{(\varphi_n)'(0)\}$. If $M_j = 0$ for all j, then it is well known that (3.25) can be strengthened to

$$|(\varphi_n)'(0)| \asymp |\lambda_n| + 1 \asymp n. \tag{3.28}$$

However, as we shall see below (also see [4]), that is not necessarily the case for $M_i > 0$.

3.2. The special case $N = 1$, $q = 0$, and Dirichlet boundary conditions

We will assume $N = 1$, $q = 0$, with Dirichlet boundary condition at $x = l$ for the remainder of this subsection. For simplicity of presentation, we also assume $M = 1$ and $l = 1$, and set $a_1 = a$. With these assumptions, it is easy to find finer spectral asymptotics than those given by Theorem 5.

Example 2. We consider the interval $(0, 1)$ with a single mass $M = 1$ placed at $a = 1/2$, and $q = 0$. The following result was proven in [19], but our proof is slightly different and serves to highlight the methods of this section. We first state some results on the spectral data that can be deduced by the methods used in the proof of Theorem 1 below. It can be shown that frequencies are all real, and after deletion of one term, can be decomposed as $\Lambda_1 \cup \Lambda_2$, with

$$\Lambda_1 := \left\{\lambda_1^{(n)}\right\} = \left\{2n\pi\right\}_1^\infty,$$
$$\Lambda_2 := \left\{\lambda_2^{(n)}\right\} = \left\{2n\pi - \frac{4}{\pi n} + O(1/n^2)\right\}_1^\infty.$$

It follows that there exists a uniform, positive spectral gap, and that the density of $\{\mu_n :\ n \in \mathbb{N}\}$ is zero. Furthermore, it follows from [21] that (3.28) holds.

We apply these results to our moment problem. It follows from [8, Theorem 3(ii)], that $\{e^{i\mu_n t} :\ n \in \mathbb{N}\}$ forms a Riesz sequence on $L^2(0, T)$ for any $T > 0$. Let $u_0 \in \mathcal{H}^{-1}$. Then it follows from (3.26) and (3.28) that $\sum_n |\alpha_n|^2 < \infty$, and so the moment problem (3.27) is solvable with control f satisfying

$$||f||^2_{L^2(0,T)} \asymp \sum_n |\alpha_n|^2 \asymp ||u_0||^2_{\mathcal{H}^{-1,D}}\ .$$

The rest of this subsection is devoted to proving Theorem 1, which we restate for the reader's convenience:

Theorem 1 *Suppose $M = N = 1$, $l = 1$, and $q = 0$. Then $R^{\mathcal{D}} = \mathcal{H}^{-1,\mathcal{D}}$ if and only if $a \in \{p/(p + 1) :\ p \in \mathbb{N}\}$.*

Here we will adopt the parametrization $(m, n) \mapsto \lambda_m^{(n)},\ m = 1, 2;\ n \in \mathbb{N}$, given by Theorem 5. In what follows, set $a = l_0,\ 1 - a = l_1$. Recall that the frequency spectrum, after deletion of one term, can be expressed as the union $\Lambda_1 \cup \Lambda_2$, with $\Lambda_m = \left\{\lambda_m^{(n)}\right\}$ satisfying

$$\lambda_m^{(n)} = \frac{n\pi}{l_m} + O(1/n). \tag{3.29}$$

Lemma 2. *The following are equivalent:*

(A) $a \in \{p/(p + 1) :\ p \in \mathbb{N}\}$,

(B) *as* $|n| \to \infty$, $dist(\lambda_2^{(n)}, \Lambda_1) \to 0$.

Proof. That (A) implies (B) follows easily by Theorem 5. Now assume (B). It follows that, after removal of one frequency, there exists $p \in \mathbb{N}$ such that

$$\lambda_2^{(n)} = \frac{pn\pi}{a} + o(1).$$

But since $\lambda_2^{(n)} = \frac{n\pi}{1-a} + O(1/n)$, we have $\frac{pn\pi}{a} = \frac{n\pi}{1-a}$. Solving for a, we conclude (A). □

In what follows, we denote by $\{\varphi_m^{(n)} : n \in \mathbb{N}\}$ the orthonormal eigenfunctions corresponding to $\lambda_m^{(n)}$.

For the purposes of our calculations, non-normalized eigenfunctions ϕ_m^n are chosen so that for $x \in (0, a)$ we have $\phi_m^n(x) = \sin(\lambda_m^{(n)} x)$, so that $(\phi_m^n)'(0) = \lambda_m^{(n)}$. Solving for ϕ_m^n on $(a, 1)$ using (2.8) and then setting $\phi_m^n(1) = 0$, we obtain the equation

$$0 = \sin\left(\lambda_m^{(n)} a\right) \cos\left(\lambda_m^{(n)}(1-a)\right) + \left(\cos\left(\lambda_m^{(n)} a\right) - \lambda \sin\left(\lambda_m^{(n)} a\right)\right) \sin\left(\lambda_m^{(n)}(1-a)\right). \tag{3.30}$$

For what follows, we will need the following sharpening of Theorem 5 which is possible given our special assumptions:

Lemma 3. *Suppose $a \in \{p/(p+1) : \; p \in \mathbb{N}\}$. Then there exists a constant $C = C(p) \neq 0$ such that the frequency spectrum decomposes into the following union:*

$$\{(p+1)\pi k : k \in \mathbb{N}\} \cup \left\{(p+1)\pi k + \frac{C}{k} + O\Big(\frac{1}{k^2}\Big) : \; k \in \mathbb{N}\right\}$$
$$\cup \left\{\frac{p+1}{p}\pi k + O\Big(\frac{1}{k}\Big) : k \in \mathbb{N}, \; k \neq mp, m \in \mathbb{N}\right\}.$$

The proof of this lemma, which is a calculus exercise applied to (3.30), resembles the proof of [19, Prop. II A.2] and is left to the reader.

Corollary 3. *Suppose $a \in \{p/(p+1) : \; p \in \mathbb{N}\}$. Let $T > 0$. Then the set of exponentials*

$$\left\{\exp(it\mu_n) : \; n \in \mathbb{N}\right\}$$

forms a Riesz sequence on $L^2(0, T)$.

We now consider the asymptotics of $\left|(\varphi_m^{(n)})'(0)\right|$, where $\{\varphi_m^{(n)}\}$ are the unit norm eigenfunctions. Since

$$(\varphi_m^{(n)})'(0) = \frac{\lambda_m^{(n)}}{\|\phi_m^n\|_{L_M^2}},$$

we will now compute $\|\phi_m^n\|_{L_M^2}$. Recall

$$||v||_{L_M^2}^2 = \int_0^a |v(x)|^2 dx + |v(a)|^2 + \int_a^1 |v(x)|^2 dx.$$

First, since $\phi_m^{(n)}(x) = \sin\left(\lambda_m^{(n)}x\right)$ on $(0,a)$, we have $\|\phi_m^n\|_{L^2_M(0,a)} \asymp 1$. Also, $\sin^2\left(\lambda_m^{(n)}a\right) = O(1)$. Solving for ϕ_m^n on $(a,1)$ using (2.8),

$$\begin{aligned}\int_a^1 |\phi_m^n|^2 &= \int_a^1 \Big| \sin\left(\lambda_m^{(n)}a\right)\cos\left(\lambda_m^{(n)}(x-a)\right) \\ &\qquad + \left(\cos\left(\lambda_m^{(n)}a\right) - \lambda_m^{(n)}\sin\left(\lambda_m^{(n)}a\right)\right)\sin\left(\lambda_m^{(n)}(x-a)\right)\Big|^2 dx \\ &= \int_a^1 \Big|\sin\left(\lambda_m^{(n)}x\right) - \lambda_m^{(n)}\sin\left(\lambda_m^{(n)}a\right)\sin\left(\lambda_m^{(n)}(x-a)\right)\Big|^2 dx.\end{aligned}$$

To estimate this last integral, we must consider separate cases.

Case i: $m = 1$**.** In this case, by (3.29),

$$\left|\lambda_1^{(n)}\sin\left(\lambda_1^{(n)}a\right)\right| = O(1). \tag{3.31}$$

Thus $\int_a^1 |\phi_m^n|^2$ is bounded as a function of n, and hence

$$\left|(\varphi_m^{(n)})'(0)\right| \asymp \left|\lambda_m^{(n)}\right| \asymp |n|, \tag{3.32}$$

from which (3.28) follows.

Case ii(a): $m = 2$ **and** $a \in \{p/(p+1):\ p \in \mathbb{N}\}$**.** In this case $l_1 = 1/(p+1)$, so we have by (3.29) that

$$\left|\lambda_2^{(n)}\sin\left(\lambda_2^{(n)}a\right)\right| = O(1).$$

We now prove the theorem in this case. Arguing as in Case i, we obtain (3.32). Also, by Corollary 3, we see

$$\left\{\exp(it\mu_n):\ n \in \mathbb{N}\right\}$$

forms a Riesz sequence in $L^2(0,T)$. Thus the moment problem (3.27) is solvable for any sequence $\{\alpha_n\} \in \ell^2$. Thus, by (3.26), the reachable set of Fourier coefficients $\{a_n(T)\}$ equals ℓ^2_{-1}, so the reachable set is $R = \mathcal{H}^{-1,\mathcal{D}}$.

Case ii(b): $m = 2$ **and** $a \neq p/(p+1)$**.** By Lemma 2, there exists a subsequence, which we will label $\{\widetilde{\lambda}_2^{(n)}\}$, of $\{\lambda_2^{(n)}\}$, and there exists $\delta > 0$ such that

$$\left|\sin\left(\widetilde{\lambda}_2^{(n)}a\right)\right| > \delta. \tag{3.33}$$

Let $\widetilde{\phi}_2^n$ be the associated eigenfunction with $(\widetilde{\phi}_2^n)'(0) = \widetilde{\lambda}_2^{(n)}$, and let $\widetilde{\varphi}_m^n$ be the associated normalized eigenfunction. We have

$$\left|\widetilde{\lambda}_2^{(n)}\sin\left(\widetilde{\lambda}_2^{(n)}a\right)\right| \asymp n.$$

Thus

$$\|\widetilde{\phi}_2^n\|_{L^2(0,1)} \asymp n,$$

and hence

$$(\widetilde{\varphi}_2^n)'(0) \asymp 1. \tag{3.34}$$

We construct an unreachable state in $H^{-1,\mathcal{D}}(0,1)$ as follows. Let $T>0$. Let $\{c^n\} \in \ell^2_{-1} \setminus \ell^2$. Let

$$v(x) = \sum_{k=1}^{\infty} c^n \widetilde{\varphi}_2^n(x).$$

It is easy to see that $v \in \mathcal{H}^{-1,\mathcal{D}} = H^{-1}(0,1)$. Furthermore, the associated moment problem (3.26) can be written

$$\frac{c^n}{(\widetilde{\varphi}_2^n)'(0)} = \langle f^T, \widetilde{e}^n \rangle,$$

where $\{\widetilde{e}^n\}$ is a Riesz sequence in $L^2(0,T)$. Clearly, this moment problem is unsolvable.

Corollary 4. *Suppose $a \in \{p/(p+1) : \ p \in \mathbb{N}\}$. Let $T>0$. For any $v \in \mathcal{H}^{-1,\mathcal{D}} = H^{-1}(0,1)$, there exists a control $f \in L^2(0,T)$ such at the solution u to the system (1.1) satisfies $u(x,T)=v(x)$ in the sense of H^{-1}, and $||f||_{L^2(0,T)} \asymp ||v||_{H^{-1}(0,T)}$.*

4. Riesz bases associated to the string equation

4.1. Divided differences

Definition 6. *Assume $\{\mu_j\}$ is a non-repeating sequence. The exponential divided difference (EDD) of order zero for $\{e^{i\mu_n t}\}$ is $[e^{i\mu_1 t}](t) := e^{i\mu_1 t}$. The EDD of order $n-1$ is given by*

$$[e^{i\mu_1 t}, \dots, e^{i\mu_n t}] = \frac{[e^{i\mu_1 t}, \dots, e^{i\mu_{n-1} t}] - [e^{i\mu_2 t}, \dots, e^{i\mu_n t}]}{\mu_1 - \mu_n}.$$

One then easily derives the formula

$$[e^{i\mu_1 t}, \dots, e^{i\mu_n t}] = \sum_{k=1}^{n} \frac{e^{i\mu_k t}}{\prod_{j\neq k}(\mu_k - \mu_j)}.$$

It is shown in [7] that the functions $[e^{i\mu_1 t}], \dots, [e^{i\mu_1 t}, \dots, e^{i\mu_n t}]$ depend on the parameters μ_j continuously and symmetrically.

Assume either Dirichlet or mixed boundary conditions at $x=l$. Recall the set of eigenfrequencies $\Lambda = \{\lambda_k : \ k \in \mathbb{N}\}$. We apply divided differences to $\left\{e^{i(\lambda_n)^2 t}\right\}$, using a partition of Λ described in [7] that we now sketch. For any $z \in \mathbb{C}$, denote by $D_z(r)$ the disk with center z and radius r. Let $G^{(p)}(r)$, $p=1,2,\dots$ be the connected components of the union $\cup_{z\in\Lambda} D_z(r)$. Write $\Lambda^{(p)}(r)$ for the subset of Λ lying in $G^{(p)}$, $\Lambda^{(p)} := \left\{\lambda_i | \lambda_i \in G_0^{(p)}(r)\right\}$. By Theorem 5, Λ can be decomposed into the union of $N+1$ uniformly discrete sets, which we label Λ_j. Let

$$\delta_j := \inf_{\gamma\neq\mu;\gamma,\mu\in\Lambda_j} |\gamma - \mu|, \quad \delta := \min_j \delta_j.$$

Then for $r < r_0 := \frac{\delta}{2N+2}$, the number $\mathcal{N}^{(p)}(r)$ of elements of $\Lambda^{(p)}$ is at most $N+1$. We now fix such r. In what follows, we refer to the sets $\Lambda^{(p)}$ as “clusters”. We use the divided difference scheme outlined above to partition Λ into clusters. In what follows, we denote the frequencies of the system (2.8) by

$$\Lambda = \{\lambda_j^p : p \in \mathbb{N}, j = 1, \dots, \mathcal{N}^{(p)}\}, \tag{4.35}$$

with φ_j^p the corresponding orthonormal eigenfunctions. In what follows, the reader should distinguish between $\{\lambda_j^p\}$, where the frequencies are partitioned according to clustering, and $\{\lambda_m^{(n)}\}$, where the partition is associated to the subintervals (a_m, a_{m+1}), $m = 0, \dots, N$. We note for future reference that we have

$$\lambda_j^p \asymp p, \quad \forall j = 1, \dots, \mathcal{N}^{(p)}.$$

Set $\mu_j^p = (\lambda_j^p)^2$. We now use the partition above to construct Exponential Divided Differences for the exponential family $\{e^{i\mu_j^p t} : p \in \mathbb{N}, j = 1, \dots, \mathcal{N}^{(p)}\}$ for the either the Dirichlet or the mixed spectrum. Thus, with $b = \mathcal{D}$ or $\mathcal{M}$, we denote

$$\mathcal{E}^b = \bigcup_{p \in \mathbb{N}} \left\{ \left[e^{i\mu_1^p t}\right], \left[e^{i\mu_1^p t}, e^{i\mu_2^p t}\right], \dots, \left[e^{i\mu_1^p t}, \dots, e^{i\mu_{\mathcal{N}^{(p)}}^p t}\right] \right\}.$$

By Theorem 5, the spectral density of $\{\mu_j^p\}$ equals zero, and so it follows from [8, Theorem 3] that for any $T > 0$, $\mathcal{E}^b$ forms Riesz sequence on $L^2(0,T)$.

We conclude this section by proving Proposition 3. Thus, assuming the Dirichlet boundary condition at $x = l$, we wish to prove

$$\#\{p : \mathcal{N}^p = N + 1\} = \infty \tag{4.36}$$

In what follows, for positive integer n, denote $\mathbf{z}^n = (z_0^n, \dots, z_N^n)$ to be a vector in $\mathbb{Z}^{N+1}$. We will construct a sequence $\{\mathbf{z}^n\}$ such that

$$\lim_{n \to \infty} \left| \frac{z_0^n}{l_0} - \frac{z_j^n}{l_j} \right| = 0, \quad j = 1, \dots, N. \tag{4.37}$$

In view of the eigenvalue asymptotics given in Theorem 5(A), this proves (4.36).

Lemma 4. *Let $\epsilon > 0$. Let U be the set of $(x_0, \dots, x_N) \in \mathbb{R}^{N+1}$ solving the system*

$$\frac{x_0}{l_0} - \frac{x_j}{l_j} < \epsilon, \quad j = 1, \dots, N. \tag{4.38}$$

Then U has the following properties:

(A) *U is open, convex, and symmetric about the origin,*
(B) *U has infinite volume.*

Proof. Part (A) is obvious. To prove part (B), consider first the system

$$\frac{x_0}{l_0} - \frac{x_j}{l_j} = 0, \quad j = 1, \dots, N.$$

We claim the solution set to this system is a one-dimensional subspace in $\mathbb{R}^{N+1}$, which we denote V. In fact, rewriting the system in matrix form, it is easy to see that the matrix has rank N, so the kernel, which is V, has dimension 1.

Since $V \subset U$, this shows U is non-empty. Let $\mathbf{v} = (v_0, \ldots, v_N)$ be a spanning vector for V. Then clearly for each j, we have $\left|\frac{v_0}{l_0} - \frac{v_j}{l_j}\right| = 0$. This implies that if $\mathbf{x} \in U$, then by (4.38) we have $\mathbf{x} + t\mathbf{v} \in U$ for any $t \in \mathbb{R}$, which means U is a cylinder in $\mathbb{R}^{N+1}$. Thus U has infinite volume, and the lemma is proved. □

We now complete the proof of the proposition. Fix $\epsilon_1 > 0$, and set $\epsilon = \epsilon_1$ in Lemma 4. We apply a theorem of Minkowski (see [11, Appendix B, Theorem 2]) to conclude there exists an integer-entry vector $\mathbf{z}^1$ in U.

Case 1: $\mathbf{z}^1 \in V$. In this case, setting $\mathbf{z}^n = n\mathbf{z}^1$, with $n \in \mathbb{N}$, we are done.

Case 2: $\mathbf{z}^1 \notin V$. In this case, let

$$\epsilon_2 = \min\left(\frac{\epsilon_1}{2}, \min_j\left(\left|\frac{z_0^1}{l_0} - \frac{z_j^1}{l_j}\right|\right)\right).$$

Let U_2 be the solution set to (4.38) with $\epsilon = \epsilon_2$. Arguing as above, there exists an integer-entry vector $\mathbf{z}^2$ in U_2.

We can now iterate this argument, using Case 1 or Case 2, to obtain a sequence $\{(\epsilon_n, \mathbf{z}^n)\}$, with ϵ_n tending to zero, and $\mathbf{z}^n$ integral solutions to (4.38) with $\epsilon = \epsilon_n$.

Proposition 3 is illustrated in Example 2 above, where $M = N = 1$, $q = 0$, and $l_0 = l_1 = 1/2$. Then Λ splits into two subsequences, $\{2\pi n\}_1^\infty$ and $\{\omega_n\}_1^\infty$, with $\omega_n = 2\pi n - \frac{4}{\pi n} + O\big(1/n^2\big)$. Thus the eigenfrequency set naturally splits into clusters of two.

5. Proof of main results

5.1. The reachable set

We begin by stating the following result.

Theorem 6. *Assume either Dirichlet or mixed boundary conditions at $x = l$. Assume 0 is not in the spectrum of A^b. Let $\left\{\lambda_j^p : p \in \mathbb{K},\ j = 1, \ldots, \mathcal{N}^{(p)}\right\}$ be the set of frequencies, with associated eigenfunctions $\left\{\varphi_j^p : p \in \mathbb{N},\ j = 1, \ldots, \mathcal{N}^{(p)}\right\}$ orthonormal with respect to L^2_M. Then for $l = 0, 1, 2, \ldots$,*

$$\left\{\sum_{j=k}^{\mathcal{N}^p} (\lambda_j^p)^{l-1} (\varphi_j^p)'(0) \varphi_j^p(x) \prod_{l=1}^{k-1} (\lambda_j^p - \lambda_l^p) \;\middle|\; p \geq 1,\ k = 1, \ldots, \mathcal{N}^{(p)}\right\}$$

forms a Riesz basis of W^b_{-l}.

Here we use the convention that

$$\prod_{j=1}^{0} (\lambda_n^p - \lambda_j^p) = 1.$$

For Dirichlet boundary conditions at $x = l$, this result was proven in [5]. However, the proof goes over with minor modifications to the case of mixed boundary condition at $x = l$. The details are left to the reader.

We wish to rewrite the moment problem (3.27) above in terms of our EDD. For λ_k^p as above and $a_1^p, \dots, a_n^p \in \mathbb{C}$, we construct divided differences of these *numbers* iteratively by $[a_1^p]' = a_1^p$, and

$$[a_1^p, \dots, a_n^p]' = \frac{[a_1^p, \dots, a_{n-1}^p]' - [a_2^p, \dots, a_n^p]'}{\mu_1^p - \mu_n^p}.$$

The following analogue of Lemma 8 in [5] holds, by the same proof as that lemma. For $n = 1, \dots, \mathcal{N}^{(p)}$,

$$a_n^p = \sum_{k=1}^{n} [a_1^p, \dots, a_k^p]' \prod_{j=1}^{k-1} \left(\mu_n^p - \mu_j^p\right).$$

Define

$$\alpha_k^p = i \frac{a_k^p(T)}{(\varphi_k^p)'(0)}.$$

We rewrite (3.27) in the form

$$[\alpha_1^p, \dots, \alpha_k^p]' = \left\langle [e_1^p, \dots, e_k^p], \overline{f}^T \right\rangle, \quad p \in \mathbb{N}, \ k = 1, \dots, \mathcal{N}^{(p)}. \tag{5.39}$$

In what follows, we write $\theta_k^p = -i\varphi_k^p(x)(\varphi_k^p)'(0)$. Thus

$$\begin{aligned} u(x,T) &= \sum_{p=1}^{\infty} \sum_{k=1}^{\mathcal{N}^{(p)}} a_k^p(T) \varphi_k^p(x) \\ &= \sum_{p=1}^{\infty} \sum_{k=1}^{\mathcal{N}^{(p)}} \alpha_k^p \theta_k^p \\ &= \sum_{p=1}^{\infty} \sum_{n=1}^{\mathcal{N}^{(p)}} \theta_n^p \sum_{k=1}^{n} [\alpha_1^p, \dots, \alpha_k^p]' \prod_{l=1}^{k-1} (\mu_j^p - \mu_l^p), \\ &= \sum_{p=1}^{\infty} \sum_{k=1}^{\mathcal{N}^{(p)}} [\alpha_1^p, \dots, \alpha_k^p]' (\sum_{j=k}^{\mathcal{N}^{(p)}} \theta_j^p \prod_{l=1}^{k-1} (\mu_j^p - \mu_l^p)). \end{aligned} \tag{5.40}$$

Since $\mathcal{E}^b$ forms a Riesz sequence of $L^2(0,T)$, it follows from (5.39) that $\left\{[\alpha_1^p, \dots, \alpha_k^p]'\right\} \in \ell^2$ if and only if $f \in L^2(0,T)$. Thus the reachable set, which we denote R^b, with b equal to $\mathcal{D}$ or $\mathcal{M}$, will be given by

$$R^b = \left\{ \sum_{p=1}^{\infty} \sum_{k=1}^{\mathcal{N}^{(p)}} c_{p,k} \left(\sum_{j=k}^{\mathcal{N}^{(p)}} \theta_j^p \prod_{l=1}^{k-1} \left(\mu_j^p - \mu_l^p\right) \right), \text{ with } c_{p,k} \in \ell^2 \right\}.$$

Thus we have the following:

Theorem 7. *Let b equal $\mathcal{M}$ or $\mathcal{D}$, and let $v \in R^b$. For any $T > 0$, there exists $f \in L^2(0,T)$ such that $u^f(x,T) = v(x)$ as elements of $\mathcal{H}^{-1,b}$. Furthermore, we* *have*

$$||f||^2_{L^2(0,T)} \asymp \sum_{p,k} \big|[\alpha_1^p, \dots, \alpha_k^p]'\big|^2.$$

Proof. We assume for now that 0 is not in the spectrum of A^b. The simple modifications in the other case will be pointed out at the end of the proof. In what follows, we use our Riesz bases to study some local properties of the functions in R^b. First,we prove Theorem 3, which we restate for the reader's convenience.

Theorem 3. *The following inclusions are valid:*

$$W^b_{-1} \subset R^b \subset \mathcal{H}^{-1,b}.$$

Furthermore, let

$$v = \sum_{p=1}^{\infty} \sum_{k=1}^{\mathcal{N}^p} c_{p,k} \left(\sum_{j=k}^{\mathcal{N}^p} \theta_j^p \prod_{l=1}^{k-1} (\mu_j^p - \mu_l^p) \right) \in R^b.$$

Then there exist positive constants C_1, C_2 such that

$$C_1 ||v||^2_{W^b_{-N-1}} \le \sum_{p=1}^{\infty} \sum_{k=1}^{\mathcal{N}^p} |c_{p,k}|^2 \le C_2 ||v||^2_{W^b_{-1}}. \tag{5.41}$$

Here $||u||^2_{W^b_{-1}}$ is possibly infinite, in which case the second inequality is vacuous.

We adopt the following notation:

$$\xi(p,k) := \sum_{j=k}^{\mathcal{N}^p} \theta_j^p \prod_{l=1}^{k-1} (\lambda_j^p - \lambda_l^p), \qquad \zeta(p,k) = \sum_{j=k}^{\mathcal{N}^p} \theta_j^p \prod_{l=1}^{k-1} \big((\lambda_j^p)^2 - (\lambda_l^p)^2\big). \tag{5.42}$$

Proof. The key is to prove some relations between the ζ and ξ. Fix p in what follows; when convenient we will drop from the notation the p dependence.

We first illustrate the computations on the simple cases $k = 1, 2$. First, recalling the convention $\prod_1^0 = 1$,

$$\xi(1) = \sum_{j=1}^{\mathcal{N}} \theta_j = \zeta(1).$$

Next, we derive a relation for $k = 2$. We have

$$\begin{aligned} \zeta(2) &= \theta_2\big((\lambda_2)^2 - (\lambda_1)^2\big) + \theta_3\big((\lambda_3)^2 - (\lambda_1)^2\big) + \cdots + \theta_{\mathcal{N}}\big((\lambda_{\mathcal{N}})^2 - (\lambda_1)^2\big) \\ &= (\lambda_2 + \lambda_1)\big(\theta_2(\lambda_2 - \lambda_1) + \theta_3(\lambda_3 - \lambda_1) + \cdots + \theta_{\mathcal{N}}(\lambda_{\mathcal{N}} - \lambda_1)\big) \\ &\quad + \big(\theta_3(\lambda_3 - \lambda_1)[(\lambda_3 + \lambda_1) - (\lambda_2 + \lambda_1)] \\ &\quad + \cdots + \theta_N(\lambda_N - \lambda_1)[(\lambda_N + \lambda_1) - (\lambda_2 + \lambda_1)]\big) \\ &= (\lambda_2 + \lambda_1)\xi(2) \\ &\quad + (\theta_3(\lambda_3 - \lambda_2)(\lambda_3 - \lambda_1) + \cdots + \theta_{\mathcal{N}}(\lambda_{\mathcal{N}} - \lambda_2)(\lambda_{\mathcal{N}} - \lambda_1)) \\ &= (\lambda_2 + \lambda_1)\xi(2) + \xi(3). \end{aligned} \tag{5.43}$$

We now exhibit the algebra that we apply for general k, starting with $k = 3$. Fix k. The zeta term corresponding to k is

$$\begin{aligned}\zeta(k) &= \left(\theta_k \prod_{l=1}^{k-1} \left((\lambda_k)^2 - (\lambda_l)^2\right) + \cdots + \theta_{\mathcal{N}} \prod_{l=1}^{k-1} \left((\lambda_{\mathcal{N}})^2 - (\lambda_l)^2\right)\right) \\ &= \left(\prod_{l=1}^{k-1} (\lambda_k + \lambda_l)\right) \xi(k) \\ &\quad + \left(\theta_{k+1} \prod_{l=1}^{k-1} (\lambda_{k+1} - \lambda_l) \left[\prod_1^{k-1} (\lambda_{k+1} + \lambda_l) - \prod_1^{k-1} (\lambda_k + \lambda_l)\right]\right. \\ &\quad \left. + \cdots + \theta_N \prod_{l=1}^{k-1} (\lambda_N - \lambda_l) \left[\prod_1^{k-1} (\lambda_N + \lambda_l) - \prod_1^{k-1} (\lambda_k + \lambda_l)\right]\right).\end{aligned}$$

For each $j > k$, $(\lambda_j - \lambda_k)$ divides $\left[\prod_1^{k-1} (\lambda_j + \lambda_l) - \prod_1^{k-1} (\lambda_k + \lambda_l)\right]$, so there exists a polynomial $P^{(k,k+1)}$ of order $(k-2)$, with coefficients depending only on k, such that the last two lines equal

$$\begin{aligned}&\left(P^{(k,k+1)}(\lambda_1, \ldots, \lambda_k, \lambda_{k+1})\ \theta_{k+1} \prod_{l=1}^{k} (\lambda_{k+1} - \lambda_l)\right. \\ &\qquad \left. + \cdots + P^{(k,k+1)}(\lambda_1, \ldots, \lambda_k, \lambda_{\mathcal{N}})\ \theta_{\mathcal{N}} \prod_{l=1}^{k} (\lambda_{\mathcal{N}} - \lambda_l)\right).\end{aligned} \tag{5.44}$$

Furthermore, there exists a polynomial $P^{(k,k+2)}$ of order $(k-3)$ such for $j = K+2, \ldots, \mathcal{N}$, we have

$$\begin{aligned}P^{(k,k+1)}&(\lambda_1, \ldots, \lambda_k, \lambda_j) - P^{(k,k+1)}(\lambda_1, \ldots, \lambda_k, \lambda_{k+1}) \\ &= (\lambda_j - \lambda_{k+1})\ P^{(k,k+2)}(\lambda_1, \ldots, \lambda_k, \lambda_{k+1}, \lambda_j).\end{aligned}$$

Thus (5.44) equals

$$\begin{aligned}&P^{(k,k+1)}(\lambda_1, \ldots, \lambda_k, \lambda_{k+1}) \xi(k+1) \\ &+ \left(P^{(k,k+2)}(\lambda_1, \ldots, \lambda_k, \lambda_{k+1}, \lambda_{k+2}) \theta_{k+2} \prod_{l=1}^{k+1} (\lambda_{k+2} - \lambda_l)\right. \\ &\left. + \cdots + P^{(k,k+2)}(\lambda_1, \ldots, \lambda_k, \lambda_{k+1}, \lambda_{\mathcal{N}}) \theta_{\mathcal{N}} \prod_{l=1}^{k+1} (\lambda_{\mathcal{N}} - \lambda_l)\right).\end{aligned}$$

In what follows, we label $P^{(k,k)} = \prod_{l=1}^{k-1} (\lambda_k + \lambda_l)$. Iterating the argument above, we get

$$\zeta(k) = \sum_{j=k}^{\mathcal{N}} P^{(k,j)} \xi(j), \tag{5.45}$$

where $P^{(k,j)}$ denotes $P^{(k,j)}(\lambda_1, \dots, \lambda_k, \dots, \lambda_j)$, and $P^{(k,j)}$ is a polynomial of degree $(2k-j-1)$ in $(\lambda_1, \dots)$.

We extend $P := P^{(k,j)}$ to an $\mathcal{N}^p \times \mathcal{N}^p$ matrix by setting $P^{k,j} = 0$ for $j < k$. Thus P is an upper triangular matrix that depends on p. The diagonal elements, which are also the eigenvalues, are by (5.45)

$$1, (\lambda_1^p + \lambda_2^p), \dots, \left(\prod_{l=1}^{\mathcal{N}^p - 1} (\lambda_{\mathcal{N}^p}^p + \lambda_l^p) \right).$$

For future reference, we define $Q = Q^{(k,j)}(p)$ to be the inverse of P. Then Q is upper-triangular and the entries to Q are bounded uniformly in p. Let $||\cdot||_*$ be the standard norm on $\mathbb{C}^{\mathcal{N}^{(p)}}$. It follows that for any $\mathbf{c} \in \mathbb{C}^{\mathcal{N}^{(p)}}$, there exists positive constant C, independent of p, such that

$$C||\mathbf{c}||_* \leq ||P\mathbf{c}||_*, \ \forall p. \tag{5.46}$$

Now suppose $u \in R^b$. Thus

$$u = \sum_p \sum_{k=1}^{\mathcal{N}^p} c_{k,p} \zeta(p,k)$$

with $\{c_{k,p}\} \in \ell^2$. Fix a p for the moment. By (5.45) we have

$$\begin{aligned} u_p := \sum_{k=1}^{\mathcal{N}} c_{p,k} \zeta(p,k) &= \sum_{k=1}^{\mathcal{N}} c_{p,k} \sum_{j=1}^{\mathcal{N}} P^{(k,j)} \xi(p,j) \\ &= \sum_{j=1}^{\mathcal{N}} \xi(p,j) \sum_{k=1}^{\mathcal{N}} c_{p,k} P^{(k,j)}. \end{aligned}$$

Since $\{\xi(p,j)\}$ forms a Riesz basis of W_{-1}^b, we have

$$\|u_p\|_{W_{-1}^b}^2 \asymp \sum_{j=1}^{\mathcal{N}} \left| \sum_{k=1}^{\mathcal{N}} c_{p,k} P^{(k,j)} \right|^2 = \left\| P^t \mathbf{c} \right\|_*^2 \geq C \sum_{k=1}^{\mathcal{N}} |c_{p,k}|^2.$$

Here P^t denotes the transpose of P, and the constant C is independent of p. Thus there exists a positive constant C such that

$$\|u\|_{W_{-1}^b}^2 \geq C \sum_p \|u_p\|_{W_{-1}^b}^2 \geq C_1 \sum_p \sum_{k=1}^{\mathcal{N}^p} |c_{p,k}|^2.$$

We now show there exists a positive constant C_2 such that

$$||u||_{W_{-N-1}^b}^2 \leq C_2 \sum_p \sum_{j=1}^{\mathcal{N}^p} |c_{p,k}|^2.$$

The details are as follows. Suppose

$$u = \sum_{p} \sum_{k=1}^{\mathcal{N}^p} c_{p,k} \zeta(p,k) \ \in R^b.$$

Fix p for the moment. Then

$$\begin{aligned} u_p = \sum_{k=1}^{\mathcal{N}} c_{p,k} \zeta(k) = \sum_{k=1}^{\mathcal{N}} c_{p,k} \sum_{j=k}^{\mathcal{N}} P^{(k,j)} \xi(j) = \sum_{j=1}^{\mathcal{N}} \xi(j) \sum_{k=1}^{j} c_{p,k} P^{(k,j)} \\ = \sum_{j=1}^{\mathcal{N}} (\lambda_j^p)^{(\mathcal{N}-1)} \xi(j) \sum_{k=1}^{\mathcal{N}} c_{p,k} P^{(k,j)} / (\lambda_j^p)^{(\mathcal{N}-1)}. \end{aligned}$$

Hence using Theorem 6, there exists positive constant C independent of p such that

$$||u_p||^2_{W^b_{-\mathcal{N}}} \leq C \sum_{j=1}^{\mathcal{N}} \left| \sum_{k=j}^{\mathcal{N}} c_{p,k} P^{(j,k)} / (\lambda_j^p)^{(\mathcal{N}-1)} \right|^2, \ \forall p.$$

By the nature of the clusters $\lambda_j^p \asymp p$, and hence it follows that $P^{(k,j)} \asymp p^{2k-j-1}$. Hence $P^{(k,j)}/(\lambda_j)^{(\mathcal{N}-1)} \asymp 1$ if $(k,j) = (\mathcal{N},\mathcal{N}) = (N+1, N+1)$ as $p \to \infty$, and $P^{(k,j)}/(\lambda_j)^{\mathcal{N}} = O(1/p)$ otherwise. Thus

$$\begin{aligned} ||u||_{W^b_{-N-1}} \leq \sum_p ||u_p||_{W^b_{-N-1}} \leq C \sum_p \left(\sum_{j=1}^{\mathcal{N}^{(p)}} \left| \sum_{k=j}^{\mathcal{N}^{(p)}} c_{p,k} P^{(k,j)} / (\lambda_j^p)^{\mathcal{N}^{(p)}} \right|^2 \right)^{1/2} \\ \leq C \left(\sum_p \sum_{k=1}^{\mathcal{N}^{(p)}} |c_{p,k}|^2 \right)^{1/2}. \end{aligned}$$

This concludes the proof of (5.41).

We now prove $W^b_{-1} \subset R^b$. The key fact, which follows easily from (5.45), is that for fixed p,

$$\xi(p,k) = \sum_{j=k}^{\mathcal{N}^p} Q^{(k,j)} \zeta(p,j). \tag{5.47}$$

Let $u := \sum_p \sum_{k=1}^{\mathcal{N}^p} d_{p,k} \xi(p,k) \in W^b_{-1}$, so $\{d_{p,k}\} \in \ell^2$. For fixed p,

$$\sum_{k=1}^{\mathcal{N}} d_{p,k} \xi(p,k) = \sum_{j=1}^{\mathcal{N}} \zeta(p,j) \sum_{k=1}^{\mathcal{N}} Q^{(k,j)} d_{p,k}.$$

Setting $c_{p,j} = \sum_{k=1}^{\mathcal{N}} Q^{(k,j)} d_{p,k}$, it is easy to check that $\sum_{p,j} |c_{p,j}|^2 < \infty$, proving $u \in R^b$.

Finally, consider the case where, say, $\lambda_1^1 = 0$. In this case, we can modify our clustering algorithm so that λ_1^1 is not clustered with any other frequency. It is not hard to show in this case that for $l \in \mathbb{N}$,

$$\varphi_1^1 \cup \left\{ \sum_{j=k}^{\mathcal{N}^p} \left(\lambda_j^p\right)^{l-1} (\varphi_j^p)'(0)\varphi_j^p(x) \prod_{l=1}^{k-1} (\lambda_j^p - \lambda_l^p) \,\Big|\, p \geq 2,\ k = 1, \dots, \mathcal{N}^{(p)} \right\}$$

forms a Riesz basis of W_{-l}^b. The proof above now applies word for word. We remark that the same modification works in the proofs below. □

The following now follows from (5.39).

Corollary 5. *Let $v \in R^b$. For any $T > 0$, there exists $f \in L^2(0,T)$ such that $u^f(x,T) = v(x)$ as elements of $H^{-1}(0,l)$. Furthermore, there exist positive constants C_1, C_2 such that*

$$C_1 ||v||^2_{W^b_{-N-1}} \leq ||f||^2_{L^2(0,T)} \leq C_2 ||v||^2_{W^b_{-1}}.$$

We now prove Proposition 2, which we restate for the reader's convenience.

Proposition 2. *Assume b equals either $\mathcal{D}$ or $\mathcal{M}$. Let $J \in \{1, \dots, N+1\}$. The condition*

$$\#\{p: \ \mathcal{N}^p \geq J\} = \infty, \tag{5.48}$$

is necessary and sufficient for there to exist

$$u \in R^b \cap \left(W^b_{-J} \setminus W^b_{-J+1}\right).$$

Proof. First we prove sufficiency. Let $\epsilon \in (0, 1/10)$. Define

$$c_{p,k} = \begin{cases} p^{-\epsilon-1/2}, & \text{if } k = J, \\ 0, & \text{otherwise.} \end{cases}$$

Thus

$$u = \sum_{p=1}^{\infty} c_{p,J}\ \theta_J^p \prod_{l=1}^{J-1} \left(\mu_J^p - \mu_l^p\right) \in R^b.$$

We have

$$u = \sum_{p=1}^{\infty} \left(c_{p,J} \prod_{l=1}^{J-1} (\lambda_J^p + \lambda_l^p) \right)\ \theta_J^p \prod_{l=1}^{J-1} (\lambda_J^p - \lambda_l^p). \tag{5.49}$$

Let l_I be the length of the shortest subinterval, and l_J the length of the longest. It is easy to see that for all p sufficiently large,

$$\frac{\pi p}{l_J} - 1 < \lambda_k^p < \frac{\pi p}{l_I} + 1, \quad \forall k \text{ such that } 1 \leq k \leq J.$$

Thus we have

$$\prod_{l=1}^{J-1} \left(\lambda_J^p + \lambda_l^p\right) \asymp p^{J-1}.$$

Thus by Theorem 6, $u \in W^b_{-J-1} \setminus W^b_{-J}$. To prove necessity, suppose $\mathcal{N}^{(p)} \geq J$ for only finitely many p. Then for any $u \in R^b$ with coefficients $\{c_{p,k}\}$, the finite sum

$$u_J := \sum_p \sum_{k=J}^{\mathcal{N}^{(p)}} c_{p,k} \sum_{j=k}^{\mathcal{N}^{(p)}} \theta_k^p \prod_{l=1}^{k-1} (\mu_j^p - \mu_l^p)$$

must be in W_1^b. It is not hard to show that $u - u_J \in W^b_{-J+1}$. In fact, since $k \leq J-1$, this follows from the estimate

$$\prod_{l=1}^{k-1} \left(\lambda_J^p + \lambda_l^p\right) < Cp^{J-2},$$

together with a factorization analogous to (5.49) and Theorem 6. □

5.2. Proofs of Corollaries 1 and 2

Assume the N masses are placed so that

$$\frac{l_j}{l_N} \in \mathbb{Q} \ \text{ and } \ \frac{l_j}{l_N} \neq \frac{2m}{2n+1}, \ \forall m, n \in \mathbb{N}, \ j = 0, \dots, N-1.$$

In this case, by Theorem 5(B), the frequencies $\{\lambda_N^{(n)}\}$ are uniformly separated from the frequency set $\{\lambda_j^{(n)} : j = 0, \dots, N-1\}$. Thus by Proposition 2, we have $R^{\mathcal{M}} \subset W^{\mathcal{M}}_{(-N)}$. This implies that for $\phi \in R^{\mathcal{M}}$, $\phi|_{(a_N, l)} \in L^2(a_N, l)$. Of course, by an analogue of Theorem 3, we also have $\phi \in \mathcal{H}^{-1,\mathcal{M}}(0, l)$.

Now we specialize to the case $N = 1$. By Theorem 3, we can conclude $R^{\mathcal{M}} = W^{\mathcal{M}}_{-1}$.

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The second Weyl coefficient for a first order system

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Abstract. For a scalar elliptic self-adjoint operator on a compact manifold without boundary we have two-term asymptotics for the number of eigenvalues between 0 and λ when $\lambda \to \infty$, under an additional dynamical condition. (See [3, Theorem 3.5] for an early result in this direction.)

In the case of an elliptic system of first order, the existence of two-term asymptotics was also established quite early and as in the scalar case Fourier integral operators have been the crucial tool. The complete computation of the coefficient of the second term was obtained only in the 2013 paper [2]. In the present paper we simplify that calculation. The main observation is that with the existence of two-term asymptotics already established, it suffices to study the resolvent as a pseudodifferential operator in order to identify and compute the second coefficient.

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1. Statement of the problem

Let A be a first order linear psedodifferential operator acting on m-columns of complex-valued half-densities over a connected closed (i.e. compact and without boundary) n-dimensional manifold M. Throughout this paper we assume that $m, n \geq 2$.

Let $A_1(x, \xi)$ and $A_{\mathrm{sub}}(x, \xi)$ be the principal and subprincipal symbols of A. Here $x = (x^1, \ldots, x^n)$ denotes local coordinates and $\xi = (\xi_1, \ldots, \xi_n)$ denotes the dual variable (momentum). The principal and subprincipal symbols are $m \times m$ matrix-functions on $T^*M \setminus \{\xi = 0\}$.

Recall that the concept of subprincipal symbol originates from the classical paper [4] of J.J. Duistermaat and L. Hörmander: see formula (5.2.8) in that paper.

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Unlike [4], we work with matrix-valued symbols, but this does not affect the formal definition of the subprincipal symbol.

We assume our operator A to be formally self-adjoint (symmetric) with respect to the standard inner product on m-columns of complex-valued half-densities, which implies that the principal and subprincipal symbols are Hermitian. We also assume that our operator A is elliptic:

$$\det A_1(x,\xi) \neq 0, \quad \forall (x,\xi) \in T^*M \setminus \{0\}. \tag{1.1}$$

Let $h^{(j)}(x,\xi)$ be the eigenvalues of the matrix-function $A_1(x,\xi)$. Throughout this paper we assume that these are simple for all $(x,\xi) \in T^*M\setminus\{0\}$. The ellipticity condition (1.1) ensures that all our $h^{(j)}(x,\xi)$ are nonzero.

We enumerate the eigenvalues of the principal symbol $h^{(j)}(x,\xi)$ in increasing order, using a positive index $j = 1,\dots,m^+$ for positive $h^{(j)}(x,\xi)$ and a negative index $j = -1,\dots,-m^-$ for negative $h^{(j)}(x,\xi)$. Here m^+ is the number of positive eigenvalues of the principal symbol and m^- is the number of negative ones. Of course, $m^+ + m^- = m$.

Let λ_k and $v_k(x)$ be the eigenvalues and the orthonormal eigenfunctions of the operator A; the particular enumeration of these eigenvalues (accounting for multiplicities) is irrelevant for our purposes. Each $v_k(x)$ is, of course, an m-column of half-densities.

Let us define the two local counting functions

$$N_\pm(x,\lambda) := \begin{cases} 0 & \text{if } \lambda \le 0, \\ \sum_{0<\pm\lambda_k<\lambda} \|v_k(x)\|^2 & \text{if } \lambda > 0. \end{cases} \tag{1.2}$$

The function $N_+(x,\lambda)$ counts the eigenvalues λ_k between zero and λ, whereas the function $N_-(x,\lambda)$ counts the eigenvalues λ_k between $-\lambda$ and zero. In both cases counting eigenvalues involves assigning them weights $\|v_k(x)\|^2$. The quantities $\|v_k(x)\|^2$ are densities on M and so are the local counting functions $N_\pm(x,\lambda)$.

Let $\hat\rho : \mathbb{R} \to \mathbb{C}$ be a smooth function such that $\hat\rho(t) = 1$ in some neighbourhood of 0 and the support of $\hat\rho$ is sufficiently small. Here 'sufficiently small' means that $\operatorname{supp}\hat\rho \subset (-\mathbf{T},\mathbf{T})$, where $\mathbf{T}$ is the infimum of the lengths of all possible loops. A loop is defined as follows. For a given j, let $(x^{(j)}(t;y,\eta),\xi^{(j)}(t;y,\eta))$ denote the Hamiltonian trajectory originating from the point (y,η), i.e. solution of the system of ordinary differential equations (the dot denotes differentiation in time t)

$$\dot x^{(j)} = h^{(j)}_\xi(x^{(j)},\xi^{(j)}), \quad \dot\xi^{(j)} = -h^{(j)}_x(x^{(j)},\xi^{(j)})$$

subject to the initial condition $(x^{(j)},\xi^{(j)})\big|_{t=0} = (y,\eta)$. Suppose that we have a Hamiltonian trajectory $(x^{(j)}(t;y,\eta),\xi^{(j)}(t;y,\eta))$ and a real number $T > 0$ such that $x^{(j)}(T;y,\eta) = y$. We say in this case that we have a loop of length T originating from the point $y \in M$.

We denote $\rho(\lambda) := \mathcal{F}^{-1}_{t\to\lambda}[\hat\rho(t)]$, where $\mathcal{F}^{-1}$ is the inverse Fourier transform. See [2, Sect. 6] for details.

Further on we will deal with the mollified counting functions $(N_\pm * \rho)(x,\lambda)$ rather than the original discontinuous counting functions $N_\pm(x,\lambda)$. Here the star stands for convolution in the variable λ. More specifically, we will deal with the derivative, in the variable λ, of the mollified counting functions. The derivative will be indicated by a prime.

It is known [1, 2, 9, 10, 11, 12, 13, 15, 16] that the functions $(N'_\pm * \rho)(x,\lambda)$ admit asymptotic expansions in integer powers of λ:

$$(N'_\pm * \rho)(x,\lambda) = a^\pm_{n-1}(x)\,\lambda^{n-1} + a^\pm_{n-2}(x)\,\lambda^{n-2} + a^\pm_{n-3}(x)\,\lambda^{n-3} + \cdots \quad \text{as } \lambda \to +\infty. \tag{1.3}$$

Definition 1.1. We call the coefficients $a^\pm_k(x)$ appearing in formula (1.3) local Weyl coefficients.

Note that our definition of Weyl coefficients does not depend on the choice of mollifier ρ.

It is also known [1, 2, 9, 10, 11, 12, 13, 15, 16] that under appropriate geometric conditions we have

$$N_\pm(x,\lambda) = \frac{a^\pm_{n-1}(x)}{n}\lambda^n + \frac{a^\pm_{n-2}(x)}{n-1}\lambda^{n-1} + o(\lambda^{n-1}) \quad \text{as } \lambda \to +\infty. \tag{1.4}$$

Remark 1.2. Our Definition 1.1 is somewhat nonstandard. It is customary to call the coefficients appearing in the asymptotic expansion (1.4) Weyl coefficients rather than those in (1.3). However, for the purposes of this paper we will stick with Definition 1.1.

Further on we deal with the coefficients $a^+_k(x)$. It is sufficient to derive formulae for the coefficients $a^+_k(x)$ because one can get formulae for $a^-_k(x)$ by replacing the operator A by the operator $-A$.

If the principal symbol of our operator A is negative definite, then the operator has a finite number of positive eigenvalues and all the coefficients $a^+_k(x)$ vanish. So further on we assume that the principal symbol has at least one positive eigenvalue. In other words, we assume that $m^+ \ge 1$.

The task at hand is to write down explicit formulae for the coefficients $a^+_{n-1}(x)$ and $a^+_{n-2}(x)$ in terms of the principal and subprincipal symbols of the operator A.

The explicit formula for the coefficient $a^+_{n-1}(x)$ has been known since at least 1980, see, for example, [9, 10, 11, 12, 13, 15, 16]. It reads

$$a^+_{n-1}(x) = \frac{n}{(2\pi)^n} \sum_{j=1}^{m^+} \int\limits_{h^{(j)}(x,\xi)<1} d\xi\,, \tag{1.5}$$

where $d\xi = d\xi_1 \cdots d\xi_n$.

The explicit formula for the coefficient $a^+_{n-2}(x)$ was derived only in 2013, see [2, formula (1.24)]. This formula reads

$$a^+_{n-2}(x) = -\frac{n(n-1)}{(2\pi)^n} \sum_{j=1}^{m^+} \int\limits_{h^{(j)}(x,\xi)<1} \Big(\big[v^{(j)}\big]^* A_{\mathrm{sub}} v^{(j)} - \frac{i}{2}\big\{ \big[v^{(j)}\big]^*, A_1 - h^{(j)}, v^{(j)} \big\} + \frac{i}{n-1} h^{(j)} \{[v^{(j)}]^*, v^{(j)}\} \Big)(x,\xi)\, d\xi\,. \tag{1.6}$$

Here curly brackets denote the Poisson bracket on matrix-functions

$$\{P,R\} := P_{x^\alpha} R_{\xi_\alpha} - P_{\xi_\alpha} R_{x^\alpha}$$

and its further generalisation

$$\{F,G,H\} := F_{x^\alpha} G H_{\xi_\alpha} - F_{\xi_\alpha} G H_{x^\alpha}\,, \tag{1.7}$$

where the subscripts x^α and ξ_α indicate partial derivatives and the repeated index α indicates summation over $\alpha = 1, \ldots, n$.

Note that if $q(x,\xi)$ is a function on $T^*M \setminus \{0\}$ positively homogeneous in ξ of degree 0, then

$$\int\limits_{h^{(j)}(x,\xi)<1} q(x,\xi)\, d\xi$$

is a density on M. Hence, the quantities (1.5) and (1.6) are densities.

The problem with the derivation of formula (1.6) given in [2] was that it was very complicated. The aim of the current paper is to provide an alternative, much simpler, derivation of formula (1.6).

It may be that the approach outlined in the current paper would allow one, in the future, to calculate further coefficients in the asymptotic expansion (1.3). Note that for an operator that is not semibounded this is a nontrivial task.

2. Strategy for the evaluation of the second Weyl coefficient

Let $z \in \mathbb{C}$, $\operatorname{Im} z > 0$. Our basic idea is to consider the resolvent $(A - zI)^{-1}$ and, by studying it, recover the second Weyl coefficient $a^+_{n-2}(x)$. Unfortunately, the operator $(A - zI)^{-1}$ is not of trace class, therefore one has to modify our basic idea so as to reduce our analysis to that of trace class operators.

Let us consider the self-adjoint operator

$$i\left[2(A - zI)^{1-n} - (A - 2zI)^{1-n} - 2(A - \bar{z}I)^{1-n} + (A - 2\bar{z}I)^{1-n}\right]. \tag{2.1}$$

We claim that the operator (2.1) is of trace class. In order to justify this claim we calculate below, for fixed z, the principal symbol of the operator (2.1) and show that it has degree of homogeneity $-n-1$.

Let B be the parametrix (approximate inverse) of A, see [18, Sect. 5] for details. Then, modulo $L^{-\infty}(M)$ (integral operators with infinitely smooth integral kernels), we have

$$\begin{aligned} A - zI &\equiv A - zAB = A(I - zB), \\ (A - zI)^{n-1} &\equiv A^{n-1}(I - zB)^{n-1}, \\ (A - zI)^{1-n} &\equiv (I - zB)^{1-n}A^{1-n} \equiv (I - zB)^{1-n}B^{n-1}. \end{aligned} \tag{2.2}$$

But

$$(I - zB)^{1-n} \equiv I + (n-1)zB - \frac{n(n-1)}{2}(zB)^2 + \cdots, \tag{2.3}$$

where the expansion is understood as an asymptotic expansion in smoothness (each subsequent term is a pseudodifferential operator of lower order). Substituting (2.3) into (2.2), we get

$$(A - zI)^{1-n} \equiv B^{n-1} + (n-1)zB^n - \frac{n(n-1)}{2}z^2B^{n+1} + \cdots. \tag{2.4}$$

Replacing z by $2z$, we get

$$(A - 2zI)^{1-n} \equiv B^{n-1} + 2(n-1)zB^n - 2n(n-1)z^2B^{n+1} + \cdots. \tag{2.5}$$

Formulae (2.4) and (2.5) imply

$$2(A - zI)^{1-n} - (A - 2zI)^{1-n} \equiv B^{n-1} + n(n-1)z^2B^{n+1} + \cdots. \tag{2.6}$$

Replacing z by $\bar{z}$, we get

$$2(A - \bar{z}I)^{1-n} - (A - 2\bar{z}I)^{1-n} \equiv B^{n-1} + n(n-1)\bar{z}^2B^{n+1} + \cdots. \tag{2.7}$$

Formulae (2.6) and (2.7) imply that the operator (2.1) is a pseudodifferential operator of order $-n-1$ with principal symbol $-4n(n-1)(\operatorname{Re} z)(\operatorname{Im} z)A_1^{-n-1}$.

It might seem more natural to consider the operator

$$(A - zI)^{-n-1} \tag{2.8}$$

instead of (2.1). The operator (2.8) is also of order $-n-1$, hence, trace class. Unfortunately, the algorithm presented in the remainder of this section won't work for the operator (2.8). The reason is that if we start with (2.8), we end up with the integral

$$\int_0^{+\infty} \frac{\mu^{n-2}}{(\mu - z)^{n+1}}\, d\mu\,, \tag{2.9}$$

where the exponent in the numerator is lower that the exponent in the denominator by more than one. The integral (2.9) is a polynomial in $\frac{1}{z}$ (no logarithm!) and it does not exhibit a jump when z crosses the positive real axis. Starting with (2.8) one can recover $a^+_{n-2} - (-1)^n a^-_{n-2}$, but it appears to be impossible to recover a^+_{n-2} itself. We need a logarithm in order to separate contributions from positive and negative eigenvalues.

The operator (2.1) is a pseudodifferential operator of order $-n-1$, hence it has a continuous integral kernel. This observation allows us to introduce the following definition.

Definition 2.1. By $f(x,z)$ we denote the real-valued continuous density obtained by restricting the integral kernel of the operator (2.1) to the diagonal $x=y$ and taking the matrix trace tr.

The explicit formula for our density is

$$f(x,z)=i\sum_{\lambda_k}\left[\frac{2}{(\lambda_k-z)^{n-1}}-\frac{1}{(\lambda_k-2z)^{n-1}}\right.\\ \left.-\frac{2}{(\lambda_k-\bar z)^{n-1}}+\frac{1}{(\lambda_k-2\bar z)^{n-1}}\right]\|v_k(x)\|^2\,. \tag{2.10}$$

This formula can be equivalently rewritten as

$$\begin{aligned} f(x,z)=i\int_0^{+\infty}&\left[\frac{2}{(\mu-z)^{n-1}}-\frac{1}{(\mu-2z)^{n-1}}\right.\\ &\left.-\frac{2}{(\mu-\bar z)^{n-1}}+\frac{1}{(\mu-2\bar z)^{n-1}}\right]N_+'(x,\mu)\,d\mu\\ &-(-1)^n\frac{2^n-1}{2^{n-1}}i\left[\frac{1}{z^{n-1}}-\frac{1}{\bar z^{n-1}}\right]\sum_{\lambda_k=0}\|v_k(x)\|^2\\ &-(-1)^n\,i\int_0^{+\infty}\left[\frac{2}{(\mu+z)^{n-1}}-\frac{1}{(\mu+2z)^{n-1}}\right.\\ &\left.-\frac{2}{(\mu+\bar z)^{n-1}}+\frac{1}{(\mu+2\bar z)^{n-1}}\right]N_-'(x,\mu)\,d\mu\,. \end{aligned} \tag{2.11}$$

The expression in the middle line of (2.11) is the contribution from the kernel (eigenspace corresponding to the eigenvalue zero) of the operator A.

Let us also introduce another density

$$\begin{aligned} f^\rho(x,z):=i\int_0^{+\infty}&\left[\frac{2}{(\mu-z)^{n-1}}-\frac{1}{(\mu-2z)^{n-1}}\right.\\ &\left.-\frac{2}{(\mu-\bar z)^{n-1}}+\frac{1}{(\mu-2\bar z)^{n-1}}\right](N_+'*\rho)(x,\mu)\,d\mu\\ -(-1)^n\,i\int_0^{+\infty}&\left[\frac{2}{(\mu+z)^{n-1}}-\frac{1}{(\mu+2z)^{n-1}}\right.\\ &\left.-\frac{2}{(\mu+\bar z)^{n-1}}+\frac{1}{(\mu+2\bar z)^{n-1}}\right](N_-'*\rho)(x,\mu)\,d\mu\,. \end{aligned} \tag{2.12}$$

Put $z=\lambda e^{i\varphi}$, where $\lambda>0$ and $0<\varphi<\pi$. We will now fix the angle φ and examine what happens when $\lambda\to+\infty$.

Lemma 2.2. *The density $f^\rho(x,\lambda e^{i\varphi})-f(x,\lambda e^{i\varphi})$ tends to zero as $\lambda\to+\infty$.*

Proof. See Appendix A. □

Lemma 2.3. *The density $f^\rho(x,\lambda e^{i\varphi})$ admits the asymptotic expansion*

$$f^\rho(x,\lambda e^{i\varphi})=b_1(x,\varphi)\lambda+b_0(x,\varphi)+o(1)\quad \text{as } \lambda\to+\infty, \tag{2.13}$$

where

$$b_1(x,\varphi) = -4(\ln 2)(n-1)(\sin\varphi)\left[a^+_{n-1}(x) + (-1)^n\, a^-_{n-1}(x)\right], \tag{2.14}$$

$$b_0(x,\varphi) = -2\left[(\pi-\varphi)\, a^+_{n-2}(x) + (-1)^n\,\varphi\, a^-_{n-2}(x)\right]. \tag{2.15}$$

Proof. See Appendices B and C. □

Lemmata 2.2 and 2.3 imply the following corollary.

Corollary 2.4. *The density* $f(x,\lambda e^{i\varphi})$ *admits the asymptotic expansion*

$$f(x,\lambda e^{i\varphi}) = b_1(x,\varphi)\lambda + b_0(x,\varphi) + o(1) \quad \text{as } \lambda\to+\infty, \tag{2.16}$$

where the coefficients $b_1(x,\varphi)$ *and* $b_0(x,\varphi)$ *are given by formulae* (2.14) *and* (2.15), *respectively.*

Suppose that we know the coefficient $b_0(x,\varphi)$ for all $\varphi\in(0,\pi)$. It is easy to see that formula (2.15) allows us to recover the second Weyl coefficient $a^+_{n-2}(x)$. Namely, if we take an arbitrary pair of distinct $\varphi_1,\varphi_2\in(0,\pi)$ then

$$a^+_{n-2}(x) = \frac{\varphi_1\, b_0(x,\varphi_2) - \varphi_2\, b_0(x,\varphi_1)}{2\pi(\varphi_2-\varphi_1)}. \tag{2.17}$$

Alternatively, the second Weyl coefficient $a^+_{n-2}(x)$ can be recovered by means of the identity

$$a^+_{n-2}(x) = -\frac{1}{2\pi}\lim_{\varphi\to0^+} b_0(x,\varphi). \tag{2.18}$$

Formulae (2.16)–(2.18) tell us that the problem of evaluating the second Weyl coefficient has been reduced to evaluating the second coefficient in the asymptotic expansion of the density $f(x,\lambda e^{i\varphi})$ as $\lambda\to+\infty$. Recall that the latter is defined in accordance with Definition 2.1.

3. The Weyl symbol of the resolvent

Let $z=\lambda e^{i\varphi}$, where $\lambda>0$ and $0<\varphi<\pi$. We formally assign to z a 'weight', as if it were positively homogeneous in ξ of degree 1. Our argument goes along the lines of [18, Sect. 9].

We performed formal calculations evaluating the symbol of the operator $(A-zI)^{-1}$ in local coordinates and then switched to the Weyl symbol. (One could have worked with Weyl symbols from the very start.) Further on we denote the Weyl symbol of the operator $(A-zI)^{-1}$ by $[(A-zI)^{-1}]_W$. We calculated $[(A-zI)^{-1}]_W$ with the two leading terms:

$$\begin{aligned}\left[(A-zI)^{-1}\right]_W &= (A_1-zI)^{-1} - (A_1-zI)^{-1}A_{\mathrm{sub}}(A_1-zI)^{-1}\\ &\quad+\frac{i}{2}\left\{(A_1-zI)^{-1}, A_1-zI, (A_1-zI)^{-1}\right\}\\ &\quad+O\left[(1+|\xi|+|z|)^{-2}(1+|\xi|)^{-1}\right].\end{aligned} \tag{3.1}$$

Here the curly brackets denote the generalised Poisson bracket on matrix functions (1.7).

The concept of a Weyl symbol was initially introduced for pseudodifferential operators in $\mathbb{R}^n$, see [18, subsection 23.3]. In the case of pseudodifferential operators acting on half-densities over a manifold it turns out that the Weyl symbol depends on the choice of local coordinates. However, in the two leading terms the Weyl symbol does not depend on the choice of local coordinates, see Appendix D. Note that a consistent definition of the full Weyl symbol for a pseudodifferential operator acting on half-densities over a manifold requires the introduction of an affine connection, see [14]. In the current paper we do not assume that we have a connection.

See Appendix E for a discussion of symbol classes and an explanation of the origins of the particular structure of the remainder term in formula (3.1), as well as remainder term estimates in subsequent formulae. In (E.22) we obtain (3.1) in the appropriate symbol classes.

Note that the expression in the second line of (3.1) can be equivalently rewritten as

$$\{(A_1-zI)^{-1},A_1-zI,(A_1-zI)^{-1}\} = (A_1-zI)^{-1}\{A_1,(A_1-zI)^{-1},A_1\}(A_1-zI)^{-1}, \tag{3.2}$$

which is the representation used by V. Ivrii, see second displayed formula on page 226 of [11]. We mention (3.2) in order to put our analysis within the context of previous research in the subject.

Let us now express the principal symbol A_1 in terms of its eigenvalues $h^{(j)}$ and eigenprojections $P^{(j)}$:

$$A_1 = \sum_j h^{(j)} P^{(j)}. \tag{3.3}$$

In what follows, we will be substituting (3.3) into our previous formulae. But before proceeding with the calculations let us discuss which expression, the one in the RHS of (3.2) or the one in the LHS of (3.2), is better suited for practical purposes. Substitution of (3.3) into the RHS of (3.2) gives a sum over five indices, whereas substitution of (3.3) into the LHS of (3.2) gives a sum over only three indices. Hence, we will stick with the representation from the LHS of (3.2).

Substituting (3.3) into (3.1), we get

$$\begin{aligned} \big[(A-zI)^{-1}\big]_W = &\sum_j \frac{P^{(j)}}{h^{(j)}-z} - \sum_{k,l} \frac{P^{(k)}A_{\mathrm{sub}}P^{(l)}}{(h^{(k)}-z)(h^{(l)}-z)} \\ &+ \frac{i}{2}\sum_{j,k,l}(h^{(j)}-z)\left\{\frac{P^{(k)}}{h^{(k)}-z}, P^{(j)}, \frac{P^{(l)}}{h^{(l)}-z}\right\} \\ &+ O\big[(1+|\xi|+|z|)^{-2}(1+|\xi|)^{-1}\big]. \end{aligned} \tag{3.4}$$

Our eigenprojections satisfy the identity

$$P^{(k)}P^{(j)} = \delta^{kj}P^{(k)}. \tag{3.5}$$

The identity (3.5) allows us to rewrite formula (3.4) as

$$\begin{aligned}
\big[(A-zI)^{-1}\big]_W &= \sum_j \frac{P^{(j)}}{h^{(j)}-z} - \sum_{k,l} \frac{P^{(k)}A_{\mathrm{sub}}P^{(l)}}{(h^{(k)}-z)(h^{(l)}-z)} \\
&\quad + \frac{i}{2}\sum_{j,k,l} \frac{h^{(j)}-z}{(h^{(k)}-z)(h^{(l)}-z)}\big\{P^{(k)},P^{(j)},P^{(l)}\big\} \\
&\quad - \frac{i}{2}\sum_{k,l} \frac{P^{(k)}\big(h^{(k)}_{x^\alpha}P^{(l)}_{\xi_\alpha} - h^{(k)}_{\xi_\alpha}P^{(l)}_{x^\alpha}\big) + \big(h^{(l)}_{\xi_\alpha}P^{(k)}_{x^\alpha} - h^{(l)}_{x^\alpha}P^{(k)}_{\xi_\alpha}\big)P^{(l)}}{(h^{(k)}-z)(h^{(l)}-z)} \\
&\quad + O\big[(1+|\xi|+|z|)^{-2}(1+|\xi|)^{-1}\big].
\end{aligned} \tag{3.6}$$

4. The matrix trace of the resolvent

Let B be a matrix pseudodifferential operator acting on m-columns of half-densities, $v \mapsto Bv$. The action of such an operator can be written in more detailed form as

$$\begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_m \end{pmatrix} \mapsto \begin{pmatrix} {B_1}^1 & {B_1}^2 & \dots & {B_1}^m \\ {B_2}^1 & {B_2}^2 & \dots & {B_2}^m \\ \vdots & \vdots & \ddots & \vdots \\ {B_m}^1 & {B_m}^2 & \dots & {B_m}^m \end{pmatrix} \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_m \end{pmatrix}, \tag{4.1}$$

where the ${B_j}^k$ are scalar pseudodifferential operators acting on half-densities.

Definition 4.1. The matrix trace of the operator (4.1) is the scalar operator

$$\operatorname{tr} B := {B_1}^1 + {B_2}^2 + \dots + {B_m}^m. \tag{4.2}$$

Obviously, the Weyl symbol of the matrix trace of an operator is the matrix trace of the Weyl symbol of the operator. Hence, formula (3.6) implies

$$\begin{aligned}
\big[\operatorname{tr}(A-zI)^{-1}\big]_W &= \sum_j \frac{1}{h^{(j)}-z} - \sum_j \frac{\operatorname{tr}\big[A_{\mathrm{sub}}P^{(j)}\big]}{(h^{(j)}-z)^2} \\
&\quad + \frac{i}{2}\sum_{j,k,l} \frac{h^{(j)}-z}{(h^{(k)}-z)(h^{(l)}-z)} \operatorname{tr}\big\{P^{(k)},P^{(j)},P^{(l)}\big\} \\
&\quad + O\big[(1+|\xi|+|z|)^{-2}(1+|\xi|)^{-1}\big].
\end{aligned} \tag{4.3}$$

Note that formula (4.3) does not contain terms with derivatives of Hamiltonians $h^{(j)}$ because all such terms cancelled out after we took the matrix trace.

Formula (3.5) implies

$$\begin{aligned}
\operatorname{tr}\big\{P^{(k)},P^{(j)},P^{(l)}\big\} &= 2\delta^{kj}\delta^{jl}\operatorname{tr}\big\{P^{(j)},P^{(j)},P^{(j)}\big\} - \delta^{kj}\operatorname{tr}\big\{P^{(l)},P^{(j)},P^{(l)}\big\} \\
&\quad - \delta^{jl}\operatorname{tr}\big\{P^{(k)},P^{(j)},P^{(k)}\big\} + \delta^{kl}\operatorname{tr}\big\{P^{(k)},P^{(j)},P^{(k)}\big\}.
\end{aligned} \tag{4.4}$$

Substituting (4.4) into (4.3) and using (3.3), we get

$$\begin{aligned}\left[\operatorname{tr}(A-zI)^{-1}\right]_W = &\sum_j \frac{1}{h^{(j)}-z} - \sum_j \frac{\operatorname{tr}\left[A_{\mathrm{sub}}P^{(j)}\right]}{(h^{(j)}-z)^2}\\ &+\frac{i}{2}\sum_j \frac{\operatorname{tr}\left\{P^{(j)},A_1-h^{(j)}I,P^{(j)}\right\}}{(h^{(j)}-z)^2} + i\sum_j \frac{\operatorname{tr}\left\{P^{(j)},P^{(j)},P^{(j)}\right\}}{h^{(j)}-z}\\ &+O\big[(1+|\xi|+|z|)^{-2}(1+|\xi|)^{-1}\big].\end{aligned} \tag{4.5}$$

Detailed calculations leading up to (4.4) and (4.5) are presented in Appendix F.

Formula (4.5) provides a compact representation for the Weyl symbol of the matrix trace of the resolvent. Even though our intermediate calculations involved summation over several (up to three) indices, summation in our final formula (4.5) is carried out over a single index.

5. The matrix trace of a power of the resolvent

In order to implement the strategy outlined in Sect. 2, we need to write down the Weyl symbol of the operator $\operatorname{tr}(A-zI)^{1-n}$.

We have the operator identity

$$(A-zI)^{1-n} = \frac{1}{(n-2)!}\,\frac{d^{n-2}}{dz^{n-2}}\,(A-zI)^{-1}\,. \tag{5.1}$$

The operations of taking the matrix trace and differentiation with respect to a parameter commute, so formula (5.1) implies

$$\operatorname{tr}(A-zI)^{1-n} = \frac{1}{(n-2)!}\,\frac{d^{n-2}}{dz^{n-2}}\,\operatorname{tr}(A-zI)^{-1}\,. \tag{5.2}$$

The latter formula, in turn, implies

$$\left[\operatorname{tr}(A-zI)^{1-n}\right]_W = \frac{1}{(n-2)!}\,\frac{d^{n-2}}{dz^{n-2}}\,[\operatorname{tr}(A-zI)^{-1}]_W\,. \tag{5.3}$$

Substituting (4.5) into (5.3), we get

$$\begin{aligned}\left[\operatorname{tr}(A-zI)^{1-n}\right]_W = &\sum_j \frac{1}{(h^{(j)}-z)^{n-1}} - (n-1)\sum_j \frac{\operatorname{tr}\left[A_{\mathrm{sub}}P^{(j)}\right]}{(h^{(j)}-z)^n}\\ &+\frac{i}{2}(n-1)\sum_j \frac{\operatorname{tr}\left\{P^{(j)},A_1-h^{(j)}I,P^{(j)}\right\}}{(h^{(j)}-z)^n}\\ &+i\sum_j \frac{\operatorname{tr}\left\{P^{(j)},P^{(j)},P^{(j)}\right\}}{(h^{(j)}-z)^{n-1}} + O\big[(1+|\xi|+|z|)^{-n}(1+|\xi|)^{-1}\big].\end{aligned} \tag{5.4}$$

We can view this as an explicit version of the result of applying $(d/dz)^{n-2}$ to the trace of (E.22) (cf. (E.39)).

6. Asymptotic expansion for the density f

We have previously defined the density $f(x,z)$, see Definition 2.1. In this section we shall derive the asymptotic expansion for the density $f(x,\lambda e^{i\varphi})$ as $\lambda\to+\infty$. The angle $0<\varphi<\pi$ will be assumed to be fixed.

Put

$$s_{1-n}^{(j)}(x,\xi,z) := \frac{1}{(h^{(j)}-z)^{n-1}}, \tag{6.1}$$

$$\begin{aligned} s_{-n}^{(j)}(x,\xi,z) := -(n-1)\frac{\operatorname{tr}\left[A_{\mathrm{sub}}P^{(j)}\right]}{(h^{(j)}-z)^{n}} + \frac{i}{2}(n-1)\frac{\operatorname{tr}\left\{P^{(j)},A_1-h^{(j)}I,P^{(j)}\right\}}{(h^{(j)}-z)^{n}} \\ + i\frac{\operatorname{tr}\left\{P^{(j)},P^{(j)},P^{(j)}\right\}}{(h^{(j)}-z)^{n-1}}, \end{aligned} \tag{6.2}$$

where the subscripts indicate the degree of homogeneity in ξ. Recall, yet again, that our convention is 'z and ξ are of the same order'. Comparing (5.4) with (6.1) and (6.2) we see that $\sum_j s_{1-n}^{(j)}$ is the leading (principal) component of the Weyl symbol of the operator $\operatorname{tr}(A-zI)^{1-n}$, whereas $\sum_j s_{-n}^{(j)}$ is the next (subprincipal) component.

The structure of formula (6.1) is very simple, whereas the structure of formula (6.2) is nontrivial. This warrants a discussion.

The first term in the RHS of (6.2) contains the expression $\operatorname{tr}[A_{\mathrm{sub}}P^{(j)}]$. It gives the 'obvious' contribution to the second Weyl coefficient. The expression $\operatorname{tr}[A_{\mathrm{sub}}P^{(j)}]$ appears in the early papers of V. Ivrii and G. V. Rozenblyum.

The second term in the RHS of (6.2) contains the expression

$$\operatorname{tr}\left\{P^{(j)},A_1-h^{(j)}I,P^{(j)}\right\}.$$

It gives a contribution to the second Weyl coefficient which is not so obvious. The expression $\operatorname{tr}\{P^{(j)},A_1-h^{(j)}I,P^{(j)}\}$ first appeared in [16].

Finally, the third term in the RHS of (6.2) contains the expression

$$\operatorname{tr}\left\{P^{(j)},P^{(j)},P^{(j)}\right\}.$$

It gives a U(1) curvature contribution to the second Weyl coefficient. This contribution to the second Weyl coefficient was identified in [2] and did not appear in previous publications.

The density $f(x,\lambda e^{i\varphi})$ is the value of the integral kernel of the operator

$$i\operatorname{tr}\left[2(A-zI)^{1-n}-(A-2zI)^{1-n}-2(A-\bar zI)^{1-n}+(A-2\bar zI)^{1-n}\right] \tag{6.3}$$

on the diagonal. We obtain the asymptotic expansion (2.16) for $f(x,\lambda e^{i\varphi})$ by replacing the operator (6.3) with its Weyl symbol and integrating in ξ. This gives the following formulae for the asymptotic coefficients:

$$b_1(x,\varphi) = \frac{1}{(2\pi)^n} \sum_j b_1^{(j)}(x,\varphi), \tag{6.4}$$

$$b_0(x,\varphi) = \frac{1}{(2\pi)^n} \sum_j b_0^{(j)}(x,\varphi), \tag{6.5}$$

where

$$\begin{aligned} b_1^{(j)}(x,\varphi) = i \int \Big[& 2s_{1-n}^{(j)}(x,\xi,e^{i\varphi}) - s_{1-n}^{(j)}(x,\xi,2e^{i\varphi}) \\ & -2s_{1-n}^{(j)}(x,\xi,e^{-i\varphi}) + s_{1-n}^{(j)}(x,\xi,2e^{-i\varphi}) \Big]\, d\xi, \end{aligned} \tag{6.6}$$

$$\begin{aligned} b_0^{(j)}(x,\varphi) = i \int \Big[& 2s_{-n}^{(j)}(x,\xi,e^{i\varphi}) - s_{-n}^{(j)}(x,\xi,2e^{i\varphi}) \\ & -2s_{-n}^{(j)}(x,\xi,e^{-i\varphi}) + s_{-n}^{(j)}(x,\xi,2e^{-i\varphi}) \Big]\, d\xi. \end{aligned} \tag{6.7}$$

The integrands in (6.6) and (6.7) decay as $|\xi|^{-n-1}$ as $|\xi| \to +\infty$, so these integrals converge.

Strictly speaking, we also have to consider the contributions from the terms $K^{(n)}$ in (E.35). However, it follows from the remark after (E.37) that they are $o(1)$ as $\lambda \to +\infty$.

7. The second Weyl coefficient

Let us us examine what happens to the integral (6.7) when $\varphi \to 0^+$. It is easy to see that if j is such that $h^{(j)} < 0$ then the integral (6.7) tends to zero as $\varphi \to 0^+$: one can simply set $\varphi = 0$ in the integrand. This means that only those j for which $h^{(j)} > 0$ contribute to the limit of the expression (6.6) when $\varphi \to 0^+$. Therefore, formulae (2.18) and (6.5) give us the following expression for the second Weyl coefficient:

$$a_{n-2}^+(x) = -\frac{1}{(2\pi)^{n+1}} \sum_{j=1}^{m^+} \lim_{\varphi \to 0^+} b_0^{(j)}(x,\varphi)\,. \tag{7.1}$$

Here the enumeration of eigenvalues of the principal symbol A_1 is assumed to be chosen in such a way that $j = 1, \ldots, m^+$ correspond to positive eigenvalues $h^{(j)}$.

It remains only to evaluate $\lim_{\varphi \to 0^+} b_0^{(j)}(x,\varphi)$ explicitly. Here $b_0^{(j)}(x,\varphi)$ is defined by formula (6.7), where the integrand is defined in accordance with (6.2).

Let us rewrite formula (6.2) as

$$s_{-n}^{(j)}(x,\xi,z) = s_{-n}^{(j;1)}(x,\xi,z) + s_{-n}^{(j;2)}(x,\xi,z), \tag{7.2}$$

where

$$s_{-n}^{(j;1)}(x,\xi,z) := -(n-1)\frac{\operatorname{tr}\left(A_{\mathrm{sub}}P^{(j)} - \frac{i}{2}\{P^{(j)}, A_1 - h^{(j)}I, P^{(j)}\}\right)}{(h^{(j)}-z)^n}, \tag{7.3}$$

$$s_{-n}^{(j;2)}(x,\xi,z) := i\frac{h^{(j)}\operatorname{tr}\{P^{(j)}, P^{(j)}, P^{(j)}\}}{h^{(j)}(h^{(j)}-z)^{n-1}}. \tag{7.4}$$

Note that the numerators in (7.3) and (7.4) are positively homogeneous in ξ of degree zero.

Formula (6.7) now reads

$$b_0^{(j)}(x,\varphi) = b_0^{(j;1)}(x,\varphi) + b_0^{(j;2)}(x,\varphi), \tag{7.5}$$

where for $k=1,2$,

$$\begin{aligned} b_0^{(j;k)}(x,\varphi) = i\int \Big[& 2s_{-n}^{(j;k)}(x,\xi,e^{i\varphi}) - s_{-n}^{(j;k)}(x,\xi,2e^{i\varphi}) \\ & -2s_{-n}^{(j;k)}(x,\xi,e^{-i\varphi}) + s_{-n}^{(j;k)}(x,\xi,2e^{-i\varphi})\Big]\,d\xi\,. \end{aligned} \tag{7.6}$$

Denote by $(S_x^*M)^{(j)}$ the $(n-1)$-dimensional unit cosphere in the cotangent fibre defined by the equation $h^{(j)}(x,\xi)=1$ and denote by $d(S_x^*M)^{(j)}$ the surface area element on $(S_x^*M)^{(j)}$ defined by the condition

$$\left[\frac{d}{d\mu}\int_{h^{(j)}(x,\xi)<\mu} g(\xi)\,d\xi\right]_{\mu=1} = \int_{(S_x^*M)^{(j)}} g(\xi)\,d(S_x^*M)^{(j)}\,, \tag{7.7}$$

where $g:\mathbb{R}^n\to\mathbb{R}$ is an arbitrary smooth function. This means that we introduce spherical coordinates in the cotangent fibre with the Hamiltonian $h^{(j)}$ playing the role of the radial coordinate, see also [17, subsection 1.1.10].

Switching to spherical coordinates, we see that each integral (7.6) is a product of two integrals, an $(n-1)$-dimensional surface integral over the unit cosphere and a 1-dimensional integral over the radial coordinate. Namely, we have

$$b_0^{(j;k)}(x,\varphi) = c^{(j;k)}(x)\,d^{(j;k)}(\varphi)\,, \tag{7.8}$$

where

$$c^{(j;1)}(x) := -(n-1)\int_{(S^*_xM)^{(j)}} \operatorname{tr}\left[A_{\mathrm{sub}}P^{(j)} - \frac{i}{2}\{P^{(j)}, A_1 - h^{(j)}I, P^{(j)}\}\right] d(S^*_xM)^{(j)}, \tag{7.9}$$

$$c^{(j;2)}(x) := i\int_{(S^*_xM)^{(j)}} h^{(j)}\operatorname{tr}\{P^{(j)}, P^{(j)}, P^{(j)}\}\, d(S^*_xM)^{(j)}, \tag{7.10}$$

$$\begin{aligned} d^{(j;1)}(\varphi) := i\int_0^{+\infty} \Bigg[&\frac{2}{(\mu - e^{i\varphi})^n} - \frac{1}{(\mu - 2e^{i\varphi})^n} \\ &- \frac{2}{(\mu - e^{-i\varphi})^n} + \frac{1}{(\mu - 2e^{-i\varphi})^n}\Bigg]\mu^{n-1}\, d\mu, \end{aligned} \tag{7.11}$$

$$\begin{aligned} d^{(j;2)}(\varphi) := i\int_0^{+\infty} \Bigg[&\frac{2}{(\mu - e^{i\varphi})^{n-1}} - \frac{1}{(\mu - 2e^{i\varphi})^{n-1}} \\ &- \frac{2}{(\mu - e^{-i\varphi})^{n-1}} + \frac{1}{(\mu - 2e^{-i\varphi})^{n-1}}\Bigg]\mu^{n-2}\, d\mu. \end{aligned} \tag{7.12}$$

Integrating by parts we see that the integrals in the right–hand-sides of (7.11) and (7.12) have the same values, i.e. they do not depend on n. Hence, it is sufficient to evaluate the integral (7.12) for $n = 2$. We have

$$\begin{aligned} d^{(j;1)}(\varphi) &= d^{(j;2)}(\varphi) \\ &= i\int_0^{+\infty}\left[\frac{2}{\mu - e^{i\varphi}} - \frac{1}{\mu - 2e^{i\varphi}} - \frac{2}{\mu - e^{-i\varphi}} + \frac{1}{\mu - 2e^{-i\varphi}}\right] d\mu \\ &= -2(\pi - \varphi)\,, \end{aligned} \tag{7.13}$$

so substituting (7.5), (7.8) and (7.13) into (7.1), we get

$$a^+_{n-2}(x) = \frac{1}{(2\pi)^n}\sum_{j=1}^{m^+}\left[c^{(j;1)}(x) + c^{(j;2)}(x)\right]. \tag{7.14}$$

Formulae (7.14), (7.9) and (7.10) give us the required explicit representation of the second Weyl coefficient. However, integrating over a unit cosphere is not very convenient, so we rewrite formulae (7.9) and (7.10) as

$$c^{(j;1)}(x) = -n(n-1)\int_{h^{(j)}(x,\xi)<1} \operatorname{tr}\left[A_{\mathrm{sub}}P^{(j)} - \frac{i}{2}\{P^{(j)}, A_1 - h^{(j)}I, P^{(j)}\}\right](x,\xi)\, d\xi, \tag{7.15}$$

$$c^{(j;2)}(x) = n\, i\int_{h^{(j)}(x,\xi)<1} \left(h^{(j)}\ \operatorname{tr}\{P^{(j)}, P^{(j)}, P^{(j)}\}\right)(x,\xi)\, d\xi\,. \tag{7.16}$$

Working with eigenprojections $P^{(j)}$ is also not very convenient, therefore we express them via the normalised eigenvectors $v^{(j)}$ of the principal symbol A_1 as

$$P^{(j)} = v^{(j)}[v^{(j)}]^*. \tag{7.17}$$

Substituting (7.17) into (7.15) and (7.16) we get

$$\begin{aligned} &c^{(j;1)}(x) \\ &= -n(n-1)\int_{h^{(j)}(x,\xi)<1} \left[[v^{(j)}]^* A_{\mathrm{sub}} v^{(j)} - \frac{i}{2}\{[v^{(j)}]^*, A_1 - h^{(j)} I, v^{(j)}\}\right](x,\xi)\, d\xi, \end{aligned} \tag{7.18}$$

$$c^{(j;2)}(x) = -n\, i \int_{h^{(j)}(x,\xi)<1} \left(h^{(j)}\, \{[v^{(j)}]^*, v^{(j)}\}\right)(x,\xi)\, d\xi\,. \tag{7.19}$$

The transition from (7.15) to (7.18) is quite straightforward, but the transition from (7.16) to (7.19) warrants an explanation. Here we have

$$\operatorname{tr}\left\{P^{(j)}, P^{(j)}, P^{(j)}\right\} = -\operatorname{tr}\left(P^{(j)}\left\{P^{(j)}, P^{(j)}\right\}\right) = -\left\{\left[v^{(j)}\right]^*, v^{(j)}\right\},$$

where at the last step we made use of [2, formula (4.17)].

The advantage of formulae (7.18) and (7.19) is that they do not involve the matrix trace.

Combining formulae (7.14), (7.18) and (7.19), we arrive at (1.6).

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Appendix A. Proof of Lemma 2.2

Let us introduce the functions

$$g_n(\mu,z) := \frac{2}{(\mu-z)^n} - \frac{1}{(\mu-2z)^n} - \text{c.c.}, \quad n\in\mathbb{N}, \quad \mu\in\mathbb{R}, \quad z\in\mathbb{C}\setminus\mathbb{R}. \tag{A.1}$$

Here and further on ‘c.c.’ stands for ‘complex conjugate terms’.

The functions (A.1) possess the following properties:

$$\partial_1 g_n(\mu,z) := \partial_\mu g_n(\mu,z) = -n g_{n+1}(\mu,z), \tag{A.2}$$

$$|g_n(\mu,z)| \le \frac{4}{|\mu-z|^n} + \frac{2}{|\mu-2z|^n}\,. \tag{A.3}$$

Formula (2.12) can be rewritten as

$$\begin{aligned} f^\rho(x,z) = i\int_0^{+\infty} g_{n-1}(\mu,z)\,(N'_+ * \rho)(x,\mu)\,d\mu \\ - (-1)^n i\int_0^{+\infty} g_{n-1}(\mu,-z)\,(N'_- * \rho)(x,\mu)\,d\mu, \end{aligned} \tag{A.4}$$

where

$$N'_\pm(x,\nu) = \sum_{\pm\lambda_k>0} \delta(\nu \mp \lambda_k)\|v_k(x)\|^2 \tag{A.5}$$

is a tempered distribution in ν supported on $\mathbb{R}_+$ and taking values in densities. The convolution

$$(N'_\pm * \rho)(x,\mu) = \int_0^{+\infty} N'_\pm(x,\nu)\,\rho(\mu-\nu)\,d\nu \tag{A.6}$$

is a continuous function of μ taking values in densities. It is known that

$$|(N'_\pm * \rho)(x,\mu)| \le c(x)(1+|\mu|^{n-1}),$$

where $c(x)$ is a fixed positive density. Arguing as in (2.2)–(2.7), it is easy to see that, for fixed z, the function $g_{n-1}(\mu,z)$ decays as $|\mu|^{-n-1}$ when $\mu\to\pm\infty$, so the integrals in (A.4) converge.

We have

$$\begin{aligned} &\int_0^{+\infty} g_{n-1}(\mu,z)\,(N'_\pm * \rho)(x,\mu)\,d\mu \\ &\qquad = \int_0^{+\infty} g_{n-1}(\mu,z)\left(\int_0^{+\infty} N'_\pm(x,\nu)\,\rho(\mu-\nu)\,d\nu\right)d\mu \\ &\qquad = \int_0^{+\infty} N'_\pm(x,\nu)\left(\int_0^{+\infty} g_{n-1}(\mu,z)\,\rho(\mu-\nu)\,d\mu\right)d\nu \\ &\qquad = \int_0^{+\infty} N'_\pm(x,\mu)\left(\int_0^{+\infty} g_{n-1}(\nu,z)\,\rho(\nu-\mu)\,d\nu\right)d\mu. \end{aligned} \tag{A.7}$$

In going from the second line of (A.7) to the third we changed the order of integration. This can be justified, for example, by replacing the infinite series (A.5) by a finite partial sum and going to the limit.

Substituting (A.7) into (A.4) and using formula (2.11), we find that

$$\begin{aligned} &f^\rho(x,z) - f(x,z) \\ &\quad = i\int_0^{+\infty} N'_+(x,\mu)\left(\int_0^{+\infty} g_{n-1}(\nu,z)\,\rho(\nu-\mu)\,d\nu - g_{n-1}(\mu,z)\right)d\mu \\ &\quad - (-1)^n i\int_0^{+\infty} N'_-(x,\mu)\left(\int_0^{+\infty} g_{n-1}(\nu,-z)\,\rho(\nu-\mu)\,d\nu - g_{n-1}(\mu,-z)\right)d\mu \\ &\quad + (-1)^n\frac{2^n-1}{2^{n-1}}i\left[\frac{1}{z^{n-1}} - \frac{1}{\bar z^{n-1}}\right]\sum_{\lambda_k=0}\|v_k(x)\|^2. \end{aligned}$$

Now, let $z = \lambda e^{i\varphi}$ with $\lambda > 0$ and fixed $\varphi \in (0, \pi)$. In view of the fact that $N_\pm(x, \lambda) = O(\lambda^n)$, in order to show that $f^\rho(x, \lambda e^{i\varphi}) - f(x, \lambda e^{i\varphi}) \to 0$ as $\lambda \to +\infty$ it is sufficient to prove that

$$\left| \int_0^{+\infty} g_{n-1}(\nu, \lambda e^{i\varphi})\, \rho(\nu - \mu)\, d\nu - g_{n-1}(\mu, \lambda e^{i\varphi}) \right| \le \frac{\mathrm{const}_\varphi}{\lambda(1 + \mu^{n+1})}\,, \ \forall \lambda \ge 1,\ \forall \mu \ge 0. \tag{A.8}$$

Recall that according to our definition of the mollifier ρ we have

$$|\rho(\nu)| \le \frac{c_p}{(1 + |\nu|)^p}\,, \quad \forall p \in \mathbb{N}, \tag{A.9}$$

$$\int_{-\infty}^{+\infty} \rho(\nu) d\nu = 1, \quad \text{and} \quad \int_{-\infty}^{+\infty} \rho(\nu) \nu^m d\nu = 0, \quad \forall m \in \mathbb{N}. \tag{A.10}$$

Formula (A.10) implies that

$$\begin{aligned} &\int_0^{+\infty} g_{n-1}(\nu, \lambda e^{i\varphi}) \rho(\nu - \mu) d\nu - g_{n-1}(\mu, \lambda e^{i\varphi}) \\ &\quad = \int_{-\infty}^{+\infty} \left[g_{n-1}(\nu, \lambda e^{i\varphi}) - g_{n-1}(\mu, \lambda e^{i\varphi}) \right] \rho(\nu - \mu) d\nu \\ &\quad - \int_{-\infty}^{0} g_{n-1}(\nu, \lambda e^{i\varphi}) \rho(\nu - \mu) d\nu. \end{aligned} \tag{A.11}$$

Using (A.3) and (A.9) with $p = n + 3$ we get

$$\begin{aligned} \left| \int_{-\infty}^{0} g_{n-1}(\nu, \lambda e^{i\varphi}) \rho(\nu - \mu) d\nu \right| &\le \int_{-\infty}^{0} \frac{6}{\lambda^{n-1} |\sin \varphi|^{n-1}} \frac{c_{n+3}}{(1 + |\nu| + \mu)^{n+3}} d\nu \\ &\le \frac{6 c_{n+3}}{\lambda^{n-1} |\sin \varphi|^{n-1} (1 + \mu^{n+1})} \int_{-\infty}^{0} \frac{d\nu}{1 + \nu^2} \\ &\le \frac{\mathrm{const}_\varphi}{\lambda(1 + \mu^{n+1})}, \quad \forall \lambda \ge 1. \end{aligned} \tag{A.12}$$

In order to estimate the first integral in the RHS of (A.11) let us perform a change of variable $\nu \mapsto \mu + \nu$,

$$\begin{aligned} &\int_{-\infty}^{+\infty} \left[g_{n-1}(\nu, \lambda e^{i\varphi}) - g_{n-1}(\mu, \lambda e^{i\varphi}) \right] \rho(\nu - \mu)\, d\nu \\ &\qquad = \int_{-\infty}^{+\infty} \left[g_{n-1}(\mu + \nu, \lambda e^{i\varphi}) - g_{n-1}(\mu, \lambda e^{i\varphi}) \right] \rho(\nu)\, d\nu. \end{aligned} \tag{A.13}$$

Writing Taylor's formula with remainder in Lagrange's form and using (A.2), we get

$$\begin{aligned} g_{n-1}(\mu+\nu,\lambda e^{i\varphi})-g_{n-1}(\mu,\lambda e^{i\varphi}) &= -(n-1)g_n(\mu,\lambda e^{i\varphi})\,\nu \\ &\quad+\frac{n(n-1)}{2}g_{n+1}(\mu,\lambda e^{i\varphi})\,\nu^2 \\ &\quad-\frac{(n+1)n(n-1)}{6}R(\mu,\nu,\lambda,\varphi)\,\nu^3, \end{aligned} \tag{A.14}$$

where

$$R(\mu,\nu,\lambda,\varphi)=g_{n+2}(\xi_{\mu,\mu+\nu},\lambda e^{i\varphi}) \tag{A.15}$$

and $\xi_{\mu,\mu+\nu}$ is some real number strictly between μ and $\mu+\nu$. From (A.10), (A.14) and (A.2), we obtain

$$\begin{aligned} &\int_{-\infty}^{+\infty}\left[g_{n-1}(\mu+\nu,\lambda e^{i\varphi})-g_{n-1}(\mu,\lambda e^{i\varphi})\right]\rho(\nu)\,d\nu \\ &\qquad=-\frac{(n+1)n(n-1)}{6}\int_{-\infty}^{+\infty}R(\mu,\nu,\lambda,\varphi)\,\nu^3\rho(\nu)\,d\nu. \end{aligned} \tag{A.16}$$

Comparing formula (A.8) with (A.11)–(A.13) and (A.16), we see that the proof of Lemma 2.2 has been reduced to proving that

$$\int_{-\infty}^{+\infty}\left|R(\mu,\nu,\lambda,\varphi)\,\nu^3\rho(\nu)\right|\,d\nu\le\frac{\mathrm{const}_\varphi}{\lambda(1+\mu^{n+1})}\,,\qquad\forall\lambda\ge1,\ \forall\mu\ge0. \tag{A.17}$$

In order to prove (A.17), it is sufficient to prove the following two estimates:

$$\int_{-\infty}^{+\infty}\left|R(\mu,\nu,\lambda,\varphi)\,\nu^3\rho(\nu)\right|\,d\nu\le\frac{\mathrm{const}_\varphi}{\lambda^{n+2}}\,,\qquad\forall\lambda\ge1,\ \forall\mu\in[0,\lambda], \tag{A.18}$$

$$\int_{-\infty}^{+\infty}\left|R(\mu,\nu,\lambda,\varphi)\,\nu^3\rho(\nu)\right|\,d\nu\le\frac{\mathrm{const}_\varphi}{\lambda\mu^{n+1}}\,,\qquad\forall\lambda\ge1,\ \forall\mu\ge\lambda. \tag{A.19}$$

Observe that formulae (A.15) and (A.3) give us the rough estimate

$$|R(\mu,\nu,\lambda,\varphi)|\le\frac{6}{|\sin\varphi|^{n+2}\lambda^{n+2}}\,,\qquad\forall\lambda>0,\ \forall\mu,\nu\in\mathbb{R}. \tag{A.20}$$

Formulae (A.20) and (A.9) with $p=5$ imply (A.18).

Formulae (A.15) and (A.3) also tell us that

$$|R(\mu,\nu,\lambda,\varphi)|\le\frac{\mathrm{const}_\varphi}{\mu^{n+2}}\le\frac{\mathrm{const}_\varphi}{\lambda\mu^{n+1}}$$

uniformly over all $\mu\ge\lambda>0$ and $\nu\ge-\mu/2$. Using this estimate and formula (A.9) with $p=5$ we get

$$\int_{-\mu/2}^{+\infty}\left|R(\mu,\nu,\lambda,\varphi)\,\nu^3\rho(\nu)\right|\,d\nu\le\frac{\mathrm{const}_\varphi}{\lambda\mu^{n+1}}\,,\qquad\forall\lambda\ge1,\ \forall\mu\ge\lambda. \tag{A.21}$$

Comparing formulae (A.21) and (A.19), we see that the proof of Lemma 2.2 has been reduced to proving that

$$\int_{-\infty}^{-\mu/2} \left|R(\mu,\nu,\lambda,\varphi)\,\nu^3\rho(\nu)\right|\,d\nu \le \frac{\mathrm{const}_\varphi}{\lambda\mu^{n+1}}\,, \quad \forall\lambda\ge 1,\ \forall\mu\ge\lambda. \tag{A.22}$$

Using (A.20) and (A.9) with $p=n+5$, we get

$$\begin{aligned}\int_{-\infty}^{-\mu/2} \left|R(\mu,\nu,\lambda,\varphi)\,\nu^3\rho(\nu)\right|\,d\nu &\le \frac{6c_{n+5}}{|\sin\varphi|^{n+2}\lambda^{n+2}}\int_{\mu/2}^{+\infty}\frac{d\nu}{\nu^{n+2}}\\ &= \frac{6\cdot 2^{n+1}c_{n+5}}{(n+1)|\sin\varphi|^{n+2}\lambda^{n+2}\mu^{n+1}}\,, \quad \forall\lambda\ge 1, \forall\mu\ge\lambda,\end{aligned}$$

which implies (A.22). □

Appendix B. Some integrals involving the functions g_n

In this appendix we evaluate some integrals involving the functions (A.1). These results will be used later in Appendix C.

Let us evaluate the following indefinite integral:

$$\begin{aligned}\int\frac{\mu^n d\mu}{(\mu-z)^n} &= \int\left(1+\frac{z}{\nu}\right)^n d\nu = \int\left[1+\frac{nz}{\nu}+\sum_{k=2}^{n}\binom{n}{k}\frac{z^k}{\nu^k}\right]d\nu\\ &= \nu + nz\log\nu + \sum_{k=2}^{n}\binom{n}{k}\frac{1}{1-k}z^k\nu^{1-k}\\ &= \mu + nz\log(\mu-z) + \sum_{k=2}^{n}\binom{n}{k}\frac{1}{1-k}z^k(\mu-z)^{1-k}.\end{aligned} \tag{B.1}$$

Here in performing intermediate calculations we used the change of variable $\nu = \mu - z$.

Similarly,

$$\begin{aligned}\int\frac{\mu^{n-1} d\mu}{(\mu-z)^n} &= \int\left(1+\frac{z}{\nu}\right)^{n-1}\frac{d\nu}{\nu} = \int\left[1+\sum_{k=1}^{n-1}\binom{n-1}{k}\frac{z^k}{\nu^k}\right]\frac{d\nu}{\nu}\\ &= \log\nu - \sum_{k=1}^{n-1}\binom{n-1}{k}\frac{1}{k}z^k\nu^{-k}\\ &= \log(\mu-z) - \sum_{k=1}^{n-1}\binom{n-1}{k}\frac{1}{k}z^k(\mu-z)^{-k}.\end{aligned} \tag{B.2}$$

Formulae (A.1), (B.1) and (B.2) imply

$$\begin{aligned}\int g_n(\mu,z)\,\mu^n\,d\mu = {}& 2nz\log(\mu-z) - 2nz\log(\mu-2z)\\ &+ 2\sum_{k=2}^{n}\binom{n}{k}\frac{1}{1-k}z^k(\mu-z)^{1-k}\\ &- \sum_{k=2}^{n}\binom{n}{k}\frac{1}{1-k}2^k z^k(\mu-2z)^{1-k} - \text{c.c.},\end{aligned} \tag{B.3}$$

$$\begin{aligned}\int g_n(\mu,z)\,\mu^{n-1}\,d\mu = {}& 2\log(\mu-z) - \log(\mu-2z)\\ &- 2\sum_{k=1}^{n-1}\binom{n-1}{k}\frac{1}{k}z^k(\mu-z)^{-k}\\ &+ \sum_{k=1}^{n-1}\binom{n-1}{k}\frac{1}{k}2^k z^k(\mu-2z)^{-k} - \text{c.c.}.\end{aligned} \tag{B.4}$$

Using (B.3) and (B.4) we can finally evaluate definite integrals:

$$\int_0^{+\infty} g_n(\mu,z)\,\mu^n\,d\mu = \left[2nz\log\left(\frac{\mu-z}{\mu-2z}\right) - 2n\bar{z}\log\left(\frac{\mu-\bar{z}}{\mu-2\bar{z}}\right)\right]\Bigg|_0^{+\infty}, \tag{B.5}$$

$$\int_0^{+\infty} g_n(\mu,z)\,\mu^{n-1}\,d\mu = \left[\log\left(\frac{\mu-z}{\mu-2z}\right) + \log\left(\frac{\mu-z}{\mu-\bar{z}}\right) - \log\left(\frac{\mu-\bar{z}}{\mu-2\bar{z}}\right)\right]\Bigg|_0^{+\infty}. \tag{B.6}$$

Here the complex logarithms are continuous multivalued functions which have to be handled carefully.

Note that for any $z\in\mathbb{C}\setminus\mathbb{R}$ and any real positive μ we have

$$\operatorname{Im}\frac{\mu-z}{\mu-2z} = \frac{\mu\operatorname{Im}z}{|\mu-2z|^2}\neq 0,$$

$$\operatorname{Im}\frac{\mu-z}{\mu-\bar{z}} = \frac{2\operatorname{Im}z(\operatorname{Re}z-\mu)}{|\mu-z|^2} = 0 \quad\Longrightarrow\quad \operatorname{Re}\frac{\mu-z}{\mu-\bar{z}} = \frac{(\operatorname{Re}z-\mu)^2-(\operatorname{Im}z)^2}{|\mu-z|^2} < 0,$$

so neither of the two arguments of our $\log$ crosses the positive real axis $\mathbb{R}_+$. Hence, we are free to switch from $\log$ to the single-valued $\operatorname{Log}:\mathbb{C}\setminus\{0\}\to\mathbb{R}+i[0,2\pi)$ branch-cut along $\mathbb{R}_+$. Formulae (B.5) and (B.6) become

$$\begin{aligned}\int_0^{+\infty} g_n(\mu,z)\,\mu^n\,d\mu &= \left[2nz\operatorname{Log}\left(\frac{\mu-z}{\mu-2z}\right) - 2n\bar{z}\operatorname{Log}\left(\frac{\mu-\bar{z}}{\mu-2\bar{z}}\right)\right]\Bigg|_0^{+\infty}\\ &= 2n(z-\bar{z})\ln 2 = 4ni(\ln 2)\operatorname{Im}z,\end{aligned} \tag{B.7}$$

$$\begin{aligned}\int_0^{+\infty} g_n(\mu,z)\,\mu^{n-1}\,d\mu &= \left[\operatorname{Log}\left(\frac{\mu-z}{\mu-2z}\right)+\operatorname{Log}\left(\frac{\mu-z}{\mu-\bar z}\right)-\operatorname{Log}\left(\frac{\mu-\bar z}{\mu-2\bar z}\right)\right]\Bigg|_0^{+\infty}\\ &= \operatorname{Log}\left(\frac{\mu-z}{\mu-\bar z}\right)\Bigg|_0^{+\infty}\\ &= i\pi(1+\operatorname{sgn}\operatorname{Im}z)-i\operatorname{Arg}z^2,\end{aligned} \tag{B.8}$$

where $\operatorname{Arg}:\mathbb{C}\setminus\{0\}\to[0,2\pi)$ is also branch-cut along $\mathbb{R}_+$.

Appendix C. Proof of Lemma 2.3

Formula (1.3) tells us that

$$(N'_\pm * \rho)(x,\mu) = a^\pm_{n-1}(x)\mu^{n-1} + a^\pm_{n-2}(x)\mu^{n-2} + (1+\mu)^{n-3}r^\pm(x,\mu), \tag{C.1}$$

where $r^\pm(x,\mu)$ is bounded uniformly in $\mu\ge 0$.

Let $g_n(\mu,z)$ be defined in accordance with (A.1). We have

$$g_n(\lambda\mu,\lambda z) = \lambda^{-n} g_n(\mu,z), \quad \forall\lambda>0. \tag{C.2}$$

Using (C.2) we get

$$\int_0^{+\infty} g_{n-1}(\mu,\lambda e^{i\varphi})\,\mu^{n-1}\,d\mu = \lambda\int_0^{+\infty} g_{n-1}(\mu,e^{i\varphi})\,\mu^{n-1}\,d\mu\,, \tag{C.3}$$

$$\int_0^{+\infty} g_{n-1}(\mu,\lambda e^{i\varphi})\,\mu^{n-2}\,d\mu = \int_0^{+\infty} g_{n-1}(\mu,e^{i\varphi})\,\mu^{n-2}\,d\mu, \tag{C.4}$$

$$\begin{aligned}&\int_0^{+\infty} g_{n-1}(\mu,\lambda e^{i\varphi})\,(1+\mu)^{n-3}\,r^\pm(x,\mu)\,d\mu\\ &= \frac{1}{\lambda}\int_0^{+\infty} g_{n-1}(\mu,e^{i\varphi})\left(\frac{1}{\lambda}+\mu\right)^{n-3} r^\pm(x,\lambda\mu)\,d\mu = o(1)\quad \text{as } \lambda\to+\infty.\end{aligned} \tag{C.5}$$

Recall (see Appendix A) that the function $g_{n-1}(\mu,z)$ decays as μ^{-n-1} when $\mu\to+\infty$, so the integrals in (C.3)–(C.5) converge.

Substituting (C.3)–(C.5) into (A.4), we get

$$\begin{aligned} f^\rho(x,\lambda e^{i\varphi}) = \lambda i\Bigg[&a^+_{n-1}(x)\int_0^{+\infty} g_{n-1}(\mu,e^{i\varphi})\,\mu^{n-1}\,d\mu\\ &-(-1)^n a^-_{n-1}(x)\int_0^{+\infty} g_{n-1}(\mu,e^{i(\varphi+\pi)})\,\mu^{n-1}\,d\mu\Bigg]\\ +\, i\Bigg[&a^+_{n-2}(x)\int_0^{+\infty} g_{n-1}(\mu,e^{i\varphi})\,\mu^{n-2}\,d\mu\\ &-(-1)^n a^-_{n-2}(x)\int_0^{+\infty} g_{n-1}(\mu,e^{i(\varphi+\pi)})\,\mu^{n-2}\,d\mu\Bigg]\\ +\, o(1)&\quad \text{as } \lambda\to+\infty.\end{aligned} \tag{C.6}$$

Formulae (B.7) and (B.8) give us the values of the integrals appearing in (C.6), so (C.6) becomes

$$f^\rho(x,\lambda e^{i\varphi}) = -\,4(n-1)(\ln 2)(\sin\varphi)\left[a^+_{n-1}(x)+(-1)^n a^-_{n-1}(x)\right]\lambda \\ -\,2\left[a^+_{n+2}(x)(\pi-\varphi)+(-1)^n a^-_{n-1}(x)\varphi\right]+o(1)\quad \text{as } \lambda\to+\infty,$$

thus proving the lemma. □

Appendix D. Weyl quantization on manifolds

Let M be a compact manifold.[1] A pseudodifferential operator of order $m \in \mathbb{R}$ is a continuous operator $A : C^\infty(M) \to C^\infty(M)$ which has a weakly continuous extension $\mathcal{D}'(M) \to \mathcal{D}'(M)$ such that, with K_A denoting the distribution kernel,

1) $\operatorname{sing\,supp} K_A \subset \operatorname{diag}(M\times M)$,
2) For every system of local coordinates $\gamma : \Omega \ni \rho \mapsto x \in \Omega' \subset \mathbb{R}^n$ where $\Omega\subset M$, $\Omega'\subset\mathbb{R}^n$ are open and γ a diffeomorphism, we have (identifying Ω and $\gamma(\Omega)$)

$$Au(x) = \frac{1}{(2\pi)^n}\iint e^{i(x-y)\cdot\theta}a(x,\theta)u(y)dyd\theta + Ru, \quad u\in C_0^\infty(\Omega),\ x\in\Omega, \tag{D.1}$$

where R is smoothing ($K_R \in C^\infty(\Omega\times\Omega)$) and a is a symbol of order m; $a\in S^m(\Omega)$, which means that $a\in C^\infty(\Omega\times\mathbb{R}^n)$ and that for every $\widehat{K}\Subset\Omega$ and all $\alpha,\beta\in\mathbb{N}^n$, $\exists C = C_{\widehat{K},\alpha,\beta}$ such that

$$|\partial_x^\alpha\partial_\theta^\beta a(x,\theta)| \le C\langle\theta\rangle^{m-|\beta|},\ \forall\,(x,\theta)\in\widehat{K}\times\mathbb{R}^n,\ \text{where } \langle\theta\rangle = (1+|\theta|^2)^{1/2}. \tag{D.2}$$

If $\widetilde{\gamma} : \widetilde{\Omega} \ni \rho \mapsto \widetilde{x} \in \widetilde{\Omega}'$ is another local coordinate chart, then over the intersection $\Omega\cap\widetilde{\Omega}$ we can express $x=\kappa(\widetilde{x})$, where $\kappa = \gamma\circ\widetilde{\gamma}^{-1}$ and we have

$$a(\kappa(\widetilde{x}),\theta) \equiv \widetilde{a}(\widetilde{x},(\kappa'(\widetilde{x}))^{\mathrm{t}}\theta) \bmod S^{m-1}. \tag{D.3}$$

This allows us to define the symbol σ_A of A on T^*M up to symbols of order 1 lower. More precisely, we have a bijection

$$L^m(M)/L^{m-1}(M) \ni A \mapsto \sigma_A \in S^m(T^*M)/S^{m-1}(T^*M), \tag{D.4}$$

with the natural definition of the symbol classes $S^m(T^*M)$, and with $L^m(M)$ denoting the space of pseudodifferential operators on M of order m.

It is well known that we can replace $a(x,\theta)$ in (D.1) with $a((x+y)/2,\theta)$ and this leads to the same definition of σ_A in $S^m/S^{m-1}(T^*M)$. Thus, working with

$$Au(x) = \operatorname{Op}(a)u(x) + Ru, \quad a\in S^m(\Omega\times\mathbf{R}^n),\ K_R\in C^\infty, \tag{D.5}$$

[1] The content of this appendix can be found in a slightly more concentrated form in the appendix of [19]. The main ideas and related results appeared earlier in Appendix a.3 in [7]. We recovered these precise references only after completing the section and decided to keep it for the convenience of the reader. See also Sect. 18.5 in [8].

leads to the same principal symbol map. Here we write[2]

$$\mathrm{Op}\,(a)u(x) = \frac{1}{(2\pi)^n} \iint e^{i(x-y)\cdot\theta} a\left(\frac{x+y}{2}, \theta\right) u(y)dyd\theta. \tag{D.6}$$

It seems to be a well-known result (though we did not find a precise reference) that if we fix a positive smooth density ω on M, restrict our attention to local coordinates for which $\omega = dx_1 \cdots dx_n$ and work with the Weyl quantization as in (D.5), (D.6), then (D.4) improves to a bijection

$$L^m/L^{m-2}(M) \ni A \mapsto \sigma_A \in S^m/S^{m-2}(T^*M). \tag{D.7}$$

A natural generalization of this is to consider pseudodifferential operators acting on 1/2-densities; $A : C^\infty(M;\Omega^{1/2}) \to C^\infty(M;\Omega^{1/2})$. When using the Weyl quantization, we get the local representation analogous to D.5:

$$A(u(y)dy^{1/2}) = (\mathrm{Op}\,(a)u)(x)dx^{1/2} + (Ru)dx^{1/2}, \tag{D.8}$$

where $dx = dx_1 \cdots dx_n$. Recall that Duistermaat and Hörmander [4] have defined invariantly the notion of subprincipal symbol of such operators when the symbols are sums of a leading positively homogeneous term of order m in ξ and a symbol of order $m-1$. This result, as well as the fixed density invariance mentioned above, follow from the next more or less well-known proposition (cf. the footnote on page 141).

Proposition D.1. *Let $L^m(M)$ denote the space of pseudodifferential operators on M of order m, acting on half-densities. Then if $(x_1, \dots, x_n)$ and $(\widetilde{x}_1, \dots, \widetilde{x}_n)$ are two local coordinate charts and we use the representation* (D.8)*, so that*

$$A(udx^{1/2}) \equiv (\mathrm{Op}\,(a)u)dx^{1/2} \equiv (\mathrm{Op}\,(\widetilde{a})\widetilde{u})d\widetilde{x}^{1/2},$$

modulo the action of smoothing operators, for $udx^{1/2} = \widetilde{u}d\widetilde{x}^{1/2}$ supported in the intersection of the two coordinate charts, then we have

$$a(\kappa(\widetilde{x}), \theta) \equiv \widetilde{a}(\widetilde{x}, \kappa'(\widetilde{x})^{\mathrm{t}}\theta) \bmod S^{m-2}, \tag{D.9}$$

implying that we have a natural bijective symbol map

$$L^m/L^{m-2}(M) \to S^m/S^{m-2}(T^*M). \tag{D.10}$$

Proof. We only verify (D.9) and omit the (even more) standard arguments for (D.10). Our proof will be a straightforward adaptation of the proof of the invariance of pseudodifferential operators under composition with diffeomorphisms by means of the Kuranishi trick (cf. [5]).

In the intersection of the two coordinate charts Ω and $\widetilde{\Omega}$, we have $u(y)dy^{1/2} = \widetilde{u}(\widetilde{y})d\widetilde{y}^{1/2}$. Here $y = \kappa(\widetilde{y})$, where κ is a diffeomorphism: $\widetilde{\gamma}(\Omega \cap \widetilde{\Omega}) \to \gamma(\Omega \cap \widetilde{\Omega})$,

[2]Strictly speaking, when Ω is not convex, we need here to insert a suitable smooth cutoff $\chi(x, y) \in C^\infty(\Omega \times \Omega)$ which is equal to one near the diagonal, the choice of which can affect the operator only by a smoothing one.

$\kappa = \gamma \circ \widetilde{\gamma}^{-1}$). Thus $u(y) = \widetilde{u}(\widetilde{y})(\det \kappa'(\widetilde{y}))^{-1/2}$, assuming that $\det \kappa' > 0$ for simplicity. Thus, modulo the action of smoothing operators

$$A(u dy^{1/2}) \equiv (\mathrm{Op}\,(a)u)dx^{1/2} = (\det \kappa'(\widetilde{x}))^{1/2}(\mathrm{Op}\,(a)u)d\widetilde{x}^{1/2},$$

so up to a smoothing operator $\mathrm{Op}\,(\widetilde{a})$ coincides with

$$B:\ \widetilde{u} \mapsto (\det \kappa'(\widetilde{x}))^{1/2}\mathrm{Op}\,(a)u, \quad u(y) = \widetilde{u}(\widetilde{y})(\det \kappa'(\widetilde{y}))^{-1/2}.$$

We have

$$\begin{aligned}
B\widetilde{u}(\widetilde{x}) &= (\det \kappa'(\widetilde{x}))^{1/2} \iint e^{i(x-y)\cdot\theta} a\left(\frac{x+y}{2}, \theta\right) u(y)dy \frac{d\theta}{(2\pi)^n} \\
&= (\det \kappa'(\widetilde{x}))^{1/2} \iint e^{i(\kappa(\widetilde{x})-y)\cdot\theta} a\left(\frac{\kappa(\widetilde{x})+y}{2}, \theta\right) \widetilde{u}(\widetilde{y})(\det \kappa'(\widetilde{y}))^{-1/2} dy \frac{d\theta}{(2\pi)^n} \\
&= \iint e^{i(\kappa(\widetilde{x})-\kappa(\widetilde{y}))\cdot\theta} a\left(\frac{\kappa(\widetilde{x})+\kappa(\widetilde{y})}{2}, \theta\right) \widetilde{u}(\widetilde{y})(\det \kappa'(\widetilde{x}) \det \kappa'(\widetilde{y}))^{1/2} d\widetilde{y} \frac{d\theta}{(2\pi)^n}.
\end{aligned}$$

By Taylor's formula (and restricting to a suitably thin neighborhood of the diagonal by means of a smooth cutoff, equal to one near the diagonal), we get

$$\kappa(\widetilde{x}) - \kappa(\widetilde{y}) = K(\widetilde{x}, \widetilde{y})(\widetilde{x} - \widetilde{y}),$$

where $\widetilde{K}(\widetilde{x}, \widetilde{y})$ depends smoothly on $(\widetilde{x}, \widetilde{y})$ and

$$K(\widetilde{x}, \widetilde{y}) = \kappa' \left(\frac{\widetilde{x}+\widetilde{y}}{2}\right) + O\big((\widetilde{x}-\widetilde{y})^2\big).$$

It follows that

$$\begin{aligned}
B\widetilde{u}(\widetilde{x}) &= \iint e^{i(\widetilde{x}-\widetilde{y})\cdot K^{\mathrm{t}}(\widetilde{x},\widetilde{y})\theta} a\left(\frac{\kappa(\widetilde{x})+\kappa(\widetilde{y})}{2}, \theta\right) \widetilde{u}(\widetilde{y})(\det \kappa'(\widetilde{x}) \det \kappa'(\widetilde{y}))^{1/2} d\widetilde{y} \frac{d\theta}{(2\pi)^n} \\
&= \iint e^{i(\widetilde{x}-\widetilde{y})\cdot\widetilde{\theta}} a\left(\frac{\kappa(\widetilde{x})+\kappa(\widetilde{y})}{2}, K^{\mathrm{t}}(\widetilde{x},\widetilde{y})^{-1}\widetilde{\theta}\right) \widetilde{u}(\widetilde{y}) \\
&\qquad \frac{(\det \kappa'(\widetilde{x}) \det \kappa'(\widetilde{y}))^{1/2}}{\det K(\widetilde{x},\widetilde{y})} d\widetilde{y} \frac{d\widetilde{\theta}}{(2\pi)^n}.
\end{aligned}$$

Here

$$\begin{aligned}
\frac{\kappa(\widetilde{x})+\kappa(\widetilde{y})}{2} &= \kappa\left(\frac{\widetilde{x}+\widetilde{y}}{2}\right) + O((\widetilde{x}-\widetilde{y})^2), \\
K^{\mathrm{t}}(\widetilde{x},\widetilde{y})^{-1} &= \left((\kappa')^{\mathrm{t}}\left(\frac{\widetilde{x}+\widetilde{y}}{2}\right)\right)^{-1} + O((\widetilde{x}-\widetilde{y})^2), \\
\det K(\widetilde{x},\widetilde{y}) &= \det \kappa'\left(\frac{\widetilde{x}+\widetilde{y}}{2}\right) + O((\widetilde{x}-\widetilde{y})^2), \\
(\det \kappa'(\widetilde{x}) \det \kappa'(\widetilde{y}))^{1/2} &= \det \kappa'\left(\frac{\widetilde{x}+\widetilde{y}}{2}\right) + O((\widetilde{x}-\widetilde{y})^2).
\end{aligned}$$

Thus,

$$B\widetilde{u} = \mathrm{Op}\,(\widetilde{a})\widetilde{u} + \iint e^{i(\widetilde{x}-\widetilde{y})\cdot\widetilde{\theta}} b(\widetilde{x},\widetilde{y},\widetilde{\theta})u(\widetilde{y})d\widetilde{y}\frac{d\widetilde{\theta}}{(2\pi)^n},$$

where $\widetilde{a} \in S^m$ is related to a as in (D.9) and $b \in S^m(\widetilde{\gamma}(\Omega\cap\widetilde{\Omega})^2 \times \mathbb{R}^n)$ (in the sense that $\partial_{\widetilde{x}}^{\alpha}\partial_{\widetilde{y}}^{\beta}\partial_{\widetilde{\theta}}^{|\delta|} b = O(\langle\widetilde{\theta}\rangle^{m-\delta})$ uniformly in $\widetilde{\theta}$ and locally uniformly in $(\widetilde{x},\widetilde{y})$) and b vanishes to the second order on the diagonal, $\widetilde{x} = \widetilde{y}$. By standard arguments we have $B \equiv \mathrm{Op}(r)$, where $r \in S^{m-2}$ and the proposition follows. □

Appendix E. The resolvent and its powers as pseudodifferential operators

Let $\gamma : M \supset \Omega \to \Omega' \subset \mathbb{R}^n$ be a chart of local coordinates and let us identify Ω' with Ω in the natural way. Let $a(x,\xi) \in S^1(\Omega\times\mathbb{R}^n)$ (defined modulo $S^{-\infty}(\Omega\times\mathbb{R}^n)$) be the Weyl symbol of

$$A_{|_{C_0^\infty(\Omega)}} : C_0^\infty(\Omega) \to C^\infty(\Omega), \tag{E.1}$$

so that

$$Au(x) = \mathrm{Op}\,(a)u(x) + Ru(x),\ \ x \in \Omega \tag{E.2}$$

for every $u \in C_0^\infty(\Omega)$, where $R \in L^{-\infty}(\Omega)$ in the sense that $K_R \in C^\infty(\Omega \times \Omega)$. Here we identify 1/2 densities and scalar functions on Ω by means of the fixed factor $dx^{1/2}$. We first work in this fixed local coordinate chart and write simply A for the operator in (E.1). We notice that

$$a - z \in S(\Omega \times \mathbb{R}^n, \langle\xi, z\rangle) = S(\langle\xi, z\rangle), \tag{E.3}$$

in the sense that $a - z \in C^\infty(\Omega \times \mathbb{R}^n)$ and that for all $K \Subset \Omega$, $\alpha, \beta \in \mathbb{N}^n$,

$$|\partial_x^\alpha \partial_\xi^\beta (a - z)| \le C_{K,\alpha,\beta}\langle\xi, z\rangle\langle\xi\rangle^{-|\beta|}, \tag{E.4}$$

uniformly when $z \in \mathbb{C}$, $|z| > 1$, $x \in K$, $\xi \in \mathbb{R}^n$. Here, we write $\langle\xi\rangle = (1 + |\xi|^2)^{1/2}$, $\langle\xi, z\rangle = (1 + |z|^2 + |\xi|^2)^{1/2}$.

Similarly, if $\Gamma \subset \dot{\mathbb{C}}$ is a closed conic neighborhood of $\dot{\mathbb{R}}$ and until further notice we restrict our attention to $z \in \dot{\mathbb{C}} \setminus (\Gamma \cup D(0, 1))$, we have

$$(a - z)^{-1} \in S(\langle\xi, z\rangle^{-1}) \tag{E.5}$$

with the natural generalization of the definition (E.4).

Sometimes, we shall exploit the fact that $a - z$ and $(a - z)^{-1}$ belong to narrower symbol classes, used in [6]. We say that $b(x, \xi, z)$, defined for (x, ξ, z) as in (E.5), belongs to $S_1(\langle\xi, z\rangle^m)$, $m \in \mathbb{R}$, if

$$|\partial_x^\alpha \partial_\xi^\beta b(x,\xi,z)| \le C_{K,\alpha,\beta} \begin{cases} \langle\xi, z\rangle^m, & \text{when } \alpha = \beta = 0, \\ \langle\xi, z\rangle^m \frac{\langle\xi\rangle}{\langle\xi,z\rangle}\langle\xi\rangle^{-|\beta|}, & \text{when } (\alpha,\beta) \ne (0,0), \end{cases} \tag{E.6}$$

uniformly for $x \in K \Subset \Omega$, $\xi \in \mathbb{R}^n$, $z \in \dot{\mathbb{C}} \setminus (\Gamma \cup D(0, 1))$.

If $b_j \in S(\langle \xi, z\rangle^{m_j})$, $j = 1, 2$, the asymptotic Weyl composition

$$\begin{aligned} b_1 \# b_2 &= \left(e^{(i/2)\sigma(D_{x,\xi};D_{y,\eta})} b_1(x,\xi) b_2(y,\eta) \right)_{\substack{y=x\\ \eta=\xi}} \\ &\sim \sum_{k=0}^{\infty} \frac{1}{k!} \left(\left(\frac{i}{2} \sigma(D_{x,\xi}; D_{y,\eta}) \right)^k b_1(x,\xi) b_2(y,\eta) \right)_{\substack{y=x\\ \eta=\xi}} \end{aligned} \tag{E.7}$$

is well defined in $S(\langle \xi, z\rangle^{m_1+m_2})/S(\langle \xi, z\rangle^{m_1+m_2}\langle \xi\rangle^{-\infty})$, where

$$S(\langle \xi, z\rangle^{m_1+m_2}\langle \xi\rangle^{-\infty}) = \bigcap_{N\geq 0} S(\langle \xi, z\rangle^{m_1+m_2}\langle \xi\rangle^{-N})$$

and with the natural definition of the symbol spaces to the right. Here

$$\sigma(D_{x,\xi}; D_{y,\eta}) = D_\xi \cdot D_y - D_x \cdot D_\eta.$$

Notice that

$$\frac{1}{k!} \left(\left(\frac{i}{2} \sigma(D_{x,\xi}; D_{y,\eta}) \right)^k b_1(x,\xi) b_2(y,\eta) \right)_{\substack{y=x\\ \eta=\xi}} \in S(\langle \xi, z\rangle^{m_1+m_2}\langle \xi\rangle^{-k}). \tag{E.8}$$

When $b_j \in S_1(m_j)$ this improves to

$$\frac{1}{k!} \left(\left(\frac{i}{2} \sigma(D_{x,\xi}; D_{y,\eta}) \right)^k b_1(x,\xi) b_2(y,\eta) \right)_{\substack{y=x\\ \eta=\xi}} \in \begin{cases} S_1(\langle \xi, z\rangle^{m_1+m_2}), & k = 0, \\ S(\langle \xi, z\rangle^{m_1+m_2-2}\langle \xi\rangle^{2-k}), & k \geq 1. \end{cases} \tag{E.9}$$

In particular,

$$b_1 \# b_2 \equiv b_1 b_2 \bmod S(\langle \xi, z\rangle^{m_1+m_2-2}\langle \xi\rangle).$$

In the special case $b_1 = a - z$, $b_2 = (a - z)^{-1}$ we get

$$(a - z)\#(a - z)^{-1} = 1 + r, \tag{E.10}$$

$$\begin{aligned} r &\sim \sum_{k=1}^{\infty} \frac{1}{k!} \left(\frac{i}{2} \sigma(D_{x,\xi}; D_{y,\eta}) \right)^k \left(a(x,\xi)(a(y,\eta) - z)^{-1} \right)_{\substack{y=x\\ \eta=\xi}} \\ &\in S(\langle \xi, z\rangle^{-2}\langle \xi\rangle)/S(\langle \xi, z\rangle^{-2}\langle \xi\rangle^{-\infty}), \\ r &\equiv \frac{i}{2} \sigma(D_{x,\xi}; D_{y,\eta}) \left(a(x,\xi)(a(y,\eta) - z)^{-1} \right)_{\substack{y=x\\ \eta=\xi}} \\ &\equiv \frac{i}{2} \{a, (a - z)^{-1}\} \bmod S(\langle \xi, z\rangle^{-2}), \end{aligned} \tag{E.11}$$

with the Poisson bracket as defined in Sect. 1.

The symbolic inverse of $A - z$ is now

$$b(x,\xi,z) \sim (a - z)^{-1}\#(1 - r + r\#r - \cdots (-1)^k r^{\#k} + \cdots), \tag{E.12}$$

where

$$r^{\#k} = \underbrace{r\#r\# \cdots \#r}_{k \text{ factors}} \in S\left((\langle \xi\rangle/\langle \xi, z\rangle^2)^k \right) \subset S\left(\langle \xi, z\rangle^{-k} \right).$$

We see that $b(x,\xi,z) \in S(\langle\xi,z\rangle^{-1})$ and that

$$b \equiv (a-z)^{-1} \bmod S\left(\frac{\langle\xi\rangle}{\langle\xi,z\rangle^3}\right).$$

More precisely,

$$b \equiv (a-z)^{-1} - (a-z)^{-1}\#r \bmod S\left(\frac{1}{\langle\xi,z\rangle^3}\right).$$

Here

$$\begin{aligned}(a-z)^{-1}\#r &\sim (a-z)^{-1}r \\ &\quad + \sum_{k\geq 1}\frac{1}{k!}\left(\left(\frac{i}{2}\sigma(D_{x,\xi};D_{y,\eta})\right)^k \left((a-z)^{-1}(x,\xi)r(y,\eta)\right)\right)_{\substack{y=x\\ \eta=\xi}} \\ &\equiv (a-z)^{-1}r \bmod S\left(\frac{1}{\langle\xi,z\rangle^3}\right),\end{aligned}$$

so

$$\begin{aligned}b(x,\xi,z) &\equiv (a-z)^{-1} - (a-z)^{-1}r \\ &\equiv (a-z)^{-1} - \frac{i}{2}(a-z)^{-1}\{a,(a-z)^{-1}\} \bmod S\left(\frac{1}{\langle\xi,z\rangle^3}\right),\end{aligned} \tag{E.13}$$

where we also used (E.11).

If $b_j \in S(\langle\xi,z\rangle^m\langle\xi\rangle^{k-j})$ for $j=0,1,\dots$, we can apply a standard procedure to construct a symbol $b \in S((\langle\xi,z\rangle^m\langle\xi\rangle^k)$ such that

$$b - \sum_0^{N-1} b_j \in S(\langle\xi,z\rangle^m\langle\xi\rangle^{k-N})$$

for every $N \geq 1$ and we still write $b \sim \sum_0^\infty b_j$ where b is a concrete symbol (uniquely determined up to $S(\langle\xi,z\rangle^m\langle\xi\rangle^{-\infty})$). If b_j are holomorphic for $z \in \dot{\mathbb{C}} \setminus (\Gamma \cup D(0,1))$, then the standard construction produces a symbol b which is also holomorphic.

If $b \in S(\langle\xi,z\rangle^m\langle\xi\rangle^k)$ is such a holomorphic symbol then by the Cauchy inequalities we get[3]

$$\partial_z^\ell b \in S(\langle\xi,z\rangle^m\langle\xi\rangle^k\langle z\rangle^{-\ell})$$

in the sense that

$$\left|\partial_x^\alpha\partial_\xi^\beta\partial_z^\ell b\right| \leq C_{K,\alpha,\beta,\ell}\langle\xi,z\rangle^m\langle\xi\rangle^{k-|\beta|}\langle z\rangle^{-\ell}$$

for $x \in K \Subset \Omega$, $\xi \in \mathbb{R}^n$ and omitting the slight increase of $\Gamma \cup D(0,1)$, mentioned in the last footnote.

[3] After replacing Γ with any closed conic set containing Γ in its interior and $D(0,1)$ with $D(0,1+\epsilon)$ for any $\epsilon > 0$

With the holomorphic z-dependence in mind we return to (E.11) and write

$$r \sim \sum_{k=1}^{\infty} r_k(x,\xi,z) \tag{E.14}$$

and get a concrete symbol $r \in S(\langle \xi, z\rangle^{-2}\langle \xi\rangle^{2-1})$ which is holomorphic in z, so that for every $N \geq 1$,

$$r - \sum_{1}^{N-1} r_k \in S(\langle \xi, z\rangle^{-2}\langle \xi\rangle^{2-N}) \tag{E.15}$$

and by the Cauchy inequalities

$$\partial_z^\ell \left(r - \sum_{1}^{N-1} r_k \right) \in S(\langle \xi, z\rangle^{-2}\langle \xi\rangle^{2-N}\langle z\rangle^{-\ell}). \tag{E.16}$$

From the explicit expression of the r_k (or from observing that they are defined for z in $(\dot{\mathbb{C}} \setminus \Gamma) \cup D(0, \langle \xi\rangle / C)$ when ξ is large), we see that

$$\partial_z^\ell r_k \in S(\langle \xi, z\rangle^{-2-\ell}\langle \xi\rangle^{2-k}), \tag{E.17}$$

$$\partial_z^\ell \left(\sum_{1}^{N-1} r_k \right) \in S(\langle \xi, z\rangle^{-2-\ell}\langle \xi\rangle^{2-1}). \tag{E.18}$$

Choosing $N = \ell + 1$ in (E.16) and (E.18), we get

$$\partial_z^\ell r \in S\big(\langle \xi, z\rangle^{-2-\ell}\langle \xi\rangle^{1}\big). \tag{E.19}$$

This shows that (E.14) is valid in the symbol space $\widetilde{S}\big(\langle \xi, z\rangle^{-2}\langle \xi\rangle^{2-1}\big)$, where we say that $c \in \widetilde{S}(\langle \xi, z\rangle^{m}\langle \xi\rangle^{k})$ if $c(x,\xi,z)$ is a smooth, holomorphic in z and

$$\partial_z^\ell c \in \widetilde{S}(\langle \xi, z\rangle^{m-\ell}\langle \xi\rangle^{k}), \text{ for all } \ell \geq 0.$$

In (E.12) we can choose $r^{\# k}$ and the asymptotic sums so that $b \in \widetilde{S}(\langle \xi, z\rangle^{-1})$ and so that (E.13) improves to

$$\begin{aligned} b(x,\xi,z) &\equiv (a-z)^{-1} - (a-z)^{-1} r \\ &\equiv (a-z)^{-1} - \frac{i}{2}(a-z)^{-1}\{a, (a-z)^{-1}\} \bmod \widetilde{S}\left(\frac{1}{\langle \xi, z\rangle^3}\right), \end{aligned} \tag{E.20}$$

where

$$r \in \widetilde{S}(\langle \xi, z\rangle^{-2}\langle \xi\rangle),\ (a-z)^{-1} \in \widetilde{S}(\langle \xi, z\rangle^{-1}). \tag{E.21}$$

In the main text we have

$$A = A_1 + A_0 + A_{-1},\ A_0 = A_{\mathrm{sub}},$$

where $A_j \in S(\langle \xi\rangle^j)$ and A_1, A_0 are positively homogeneous in ξ of degree 1 and 0 respectively, in the region $|\xi| \geq 1$. From the resolvent identity

$$\begin{aligned} (a-z)^{-1} = (A_1 - z)^{-1} &- (A_1-z)^{-1}(a-A_1)(A_1-z)^{-1} \\ &+ (A_1-z)^{-1}(a-A_1)(a-z)^{-1}(a-A_1)(A_1-z)^{-1} \end{aligned}$$

we infer that

$$(a-z)^{-1} \equiv (A_1-z)^{-1} - (A_1-z)^{-1}(A_0+A_{-1})(A_1-z)^{-1} \bmod \widetilde{S}(\langle \xi, z\rangle^{-3}),$$

hence,

$$(a-z)^{-1} \equiv (A_1-z)^{-1} - (A_1-z)^{-1}A_0(A_1-z)^{-1} \bmod \widetilde{S}(\langle \xi\rangle^{-1}\langle \xi, z\rangle^{-2}).$$

In particular,

$$(a-z)^{-1} \equiv (A_1-z)^{-1} \bmod \widetilde{S}(\langle \xi, z\rangle^{-2})$$

and from (E.20) we get

$$\begin{aligned} b \equiv (A_1-z)^{-1} &- (A_1-z)^{-1}A_0(A_1-z)^{-1} \\ &- \frac{i}{2}(A_1-z)^{-1}\{A_1,(A_1-z)^{-1}\} \bmod \widetilde{S}\left(\frac{1}{\langle\xi\rangle\langle \xi, z\rangle^2}\right), \end{aligned} \tag{E.22}$$

which implies (3.1) (cf. (3.2)).

By construction, b is a realization of the symbolic inverse of $a-z$:

$$(a-z)\#b \equiv 1 \bmod \widetilde{S}(\langle \xi, z\rangle^{-2}\langle\xi\rangle^{-\infty}).$$

Let $B = \mathrm{Op}\,(b) : C_0^\infty(\Omega) \to C^\infty(\Omega)$ (where we also insert a suitable cutoff $\in C^\infty(\Omega\times\Omega)$, equal to 1 near $\mathrm{diag}\,(\Omega\times\Omega)$). Then

$$\partial_z^k B(z) = O(\langle z\rangle^{-k_1}) : H^s_{\mathrm{comp}}(\Omega) \to H^{s+k_2}_{\mathrm{loc}}(\Omega) \text{ uniformly for } z \in \dot{\mathbb{C}}\setminus(\Gamma\cup D(0,1)), \tag{E.23}$$

when $1+k = k_1+k_2$, $k_j \geq 0$, $s\in\mathbb{R}$.

Let $\chi,\Phi \in C_0^\infty(\Omega)$, with $\Phi = 1$ near $\mathrm{supp}\,(\chi)$. Then,

$$(A-z)\Phi B\chi = \chi + R, \tag{E.24}$$

where $R = R(z)$ is a smoothing operator: $\mathcal{D}'(\Omega) \to C^\infty(\Omega)$, depending holomorphically on z, such that $Ru = 0$ when $\mathrm{supp}\,(u)\cap\mathrm{supp}\,(\chi) = \emptyset$ and

$$\partial_z^k R = O(\langle z\rangle^{-2-k}) : H^{-s}(\Omega) \to H^s_{\mathrm{loc}}(\Omega),\ z \in \dot{\mathbb{C}}\setminus(\Gamma\cup D(0,1)), \tag{E.25}$$

for all $s\in\mathbb{R}$, $k\geq 0$. We omit the standard proof of this, based on the symbolic results above, starting with the identity

$$(A-z)\Phi B\chi = [A,\Phi]B\chi + \Phi(A-z)B\chi.$$

Let $M \subset \bigcup_1^N \Omega_j$ be a finite covering of M with coordinate charts as above. Recall that A is a globally defined pseudodifferential operator acting on 1/2-densities so we can now view $A-z$ as acting: $C_0^\infty(\Omega_j;\Omega^{1/2}) \to C^\infty(M;\Omega^{1/2})$ for each j. We have a corresponding operator B_j (as "B" above), now acting on 1/2-densities, so that

$$B_j(u dx^{1/2}) = (\mathrm{Op}\,(b_j)u)dx^{1/2},\ u \in C_0^\infty(\Omega_j) \tag{E.26}$$

where $dx^{1/2}$ is the canonical (and j-dependent) 1/2-density on Ω_j. Let $\chi_j \in C_0^\infty(\Omega_j)$ form a partition of unity on M. Equation (E.24) becomes

$$(A-z)\Phi_j B_j\chi_j = \chi_j + R_j(z), \tag{E.27}$$

where R_j has the properties of "R" in (E.23), (E.25) except for the fact that R_j acts on 1/2-densities and that we can actually define R_j as an operator on M such that

$$\|\partial_z^k R_j\|_{\mathcal{L}(H^{-s},H^s(M))} \leq C_s\langle z\rangle^{-2-k},\ z \in \dot{\mathbb{C}} \setminus (\Gamma \cup D(0,1)). \tag{E.28}$$

Here $H^s(M)$ denotes the Sobolev space of 1/2-densities of order $s \in \mathbb{R}$.

Let

$$B := \sum \Phi_j B_j \chi_j :\ C^\infty(M;\Omega^{1/2}) \to C^\infty(M;\Omega^{1/2}). \tag{E.29}$$

Then

$$(A-z)B(z) = 1 + R(z), \tag{E.30}$$

$$R(z) = \sum R_j(z), \tag{E.31}$$

$$\partial_z^k B(z) = O(\langle z\rangle^{-k_1}) :\ H^s \to H^{s+k_2},\ \text{when } k+1 = k_1 + k_2,\ k_j \geq 0, \tag{E.32}$$

$$\partial_z^k R(z) = O_s(\langle z\rangle^{-2-k}) :\ H^{-s} \to H^s, \tag{E.33}$$

for all $s \in \mathbb{R}$.

On the other hand, by direct arguments, we know that $(A-z)^{-1}$ also enjoys the properties (E.32). Applying this operator to the left in (E.30), we get

$$(A-z)^{-1} = B(z) - K(z),\ K(z) = (A-z)^{-1}R(z). \tag{E.34}$$

Clearly, $K(z)$ also satisfies (E.33).

Using the operator identity (5.1) in (E.34), we get

$$(A-z)^{1-n} = B^{(n)}(z) - K^{(n)}(z), \tag{E.35}$$

$$B^{(n)} = \frac{1}{(n-2)!}\partial_z^{n-2}B(z), \tag{E.36}$$

$$K^{(n)} = \frac{1}{(n-2)!}\partial_z^{n-2}K(z) = O_s(\langle z\rangle^{-n}) :\ H^{-s} \to H^s. \tag{E.37}$$

From the last estimate it follows that $K^{(n)}$ is of trace class with a continuous distribution kernel which is uniformly $= O(\langle z\rangle^{-n})$.

Let x_0 be a point in a coordinate chart $\Omega = \Omega_j$ and assume for simplicity that $\chi = \chi_j$ is equal to 1 near that point. Then near (x_0, x_0) the distribution kernel of B (identified locally with an operator acting on scalar functions) coincides with that of $\mathrm{Op}\,(b)$, where b satisfies (E.20). Consequently,

$$B^{(n)} = \mathrm{Op}\,(b^{(n)}), \tag{E.38}$$

$$b^{(n)} \equiv (a-z)^{-n} - \frac{1}{(n-2)!}\partial_z^{n-2}\left((a-z)^{-1}r\right) \mod \widetilde{S}\left(\langle \xi, z\rangle^{-n-1}\right). \tag{E.39}$$

Appendix F. Proof of formulae (4.4) and (4.5)

Formula (3.5) implies

$$(\partial P^{(k)})P^{(j)} + P^{(k)}\partial P^{(j)} = \delta^{kj}\partial P^{(k)}, \tag{F.1}$$

where ∂ is any partial derivative. We have

$$\begin{aligned}\operatorname{tr}\{P^{(k)}, P^{(j)}, P^{(l)}\} &= \operatorname{tr}\bigl[(\partial_{x^\alpha}P^{(k)})P^{(j)}\partial_{\xi_\alpha}P^{(l)} - (\partial_{\xi_\alpha}P^{(k)})P^{(j)}\partial_{x^\alpha}P^{(l)}\bigr]\\ &= \operatorname{tr}\bigl[\bigl((\partial_{x^\alpha}P^{(k)})P^{(j)}\bigr)\bigl(P^{(j)}\partial_{\xi_\alpha}P^{(l)}\bigr)\\ &\quad - \bigl((\partial_{\xi_\alpha}P^{(k)})P^{(j)}\bigr)\bigl(P^{(j)}\partial_{x^\alpha}P^{(l)}\bigr)\bigr].\end{aligned}$$

Using (F.1), we can rewrite the above formula as

$$\begin{aligned}\operatorname{tr}\{P^{(k)}, P^{(j)}, P^{(l)}\} = \operatorname{tr}\bigl[&\bigl(\delta^{kj}\partial_{x^\alpha}P^{(j)} - P^{(k)}\partial_{x^\alpha}P^{(j)}\bigr)\bigl(\delta^{jl}\partial_{\xi_\alpha}P^{(j)} - (\partial_{\xi_\alpha}P^{(j)})P^{(l)}\bigr)\\ &- \bigl(\delta^{kj}\partial_{\xi_\alpha}P^{(j)} - P^{(k)}\partial_{\xi_\alpha}P^{(j)}\bigr)\bigl(\delta^{jl}\partial_{x^\alpha}P^{(j)} - (\partial_{x^\alpha}P^{(j)})P^{(l)}\bigr)\bigr].\end{aligned}$$

Expanding the parentheses in the above formula and rearranging terms, we get

$$\begin{aligned}\operatorname{tr}\{P^{(k)}, P^{(j)}, P^{(l)}\} = \delta^{kj}\operatorname{tr}\{P^{(j)}, P^{(l)}, P^{(j)}\} &+ \delta^{jl}\operatorname{tr}\{P^{(j)}, P^{(k)}, P^{(j)}\}\\ &- \delta^{kl}\operatorname{tr}\{P^{(j)}, P^{(k)}, P^{(j)}\}.\end{aligned} \tag{F.2}$$

In the special case $l = k$, the above formula becomes

$$\operatorname{tr}\{P^{(k)}, P^{(j)}, P^{(k)}\} = 2\delta^{kj}\operatorname{tr}\{P^{(j)}, P^{(j)}, P^{(j)}\} - \operatorname{tr}\{P^{(j)}, P^{(k)}, P^{(j)}\}. \tag{F.3}$$

Each of the three terms in the RHS of (F.2) can now be rewritten using the identity (F.3) with appropriate choice of indices, which gives us (4.4).

Let us now substitute (4.4) into the triple sum in the RHS of (4.3):

$$\begin{aligned}
&\sum_{j,k,l} \frac{h^{(j)}-z}{(h^{(k)}-z)(h^{(l)}-z)} \operatorname{tr}\{P^{(k)},P^{(j)},P^{(l)}\} \\
&= 2\sum_j \frac{1}{h^{(j)}-z}\operatorname{tr}\{P^{(j)},P^{(j)},P^{(j)}\} - \sum_{j,l}\frac{1}{h^{(l)}-z}\operatorname{tr}\{P^{(l)},P^{(j)},P^{(l)}\} \\
&\quad - \sum_{j,k}\frac{1}{h^{(k)}-z}\operatorname{tr}\{P^{(k)},P^{(j)},P^{(k)}\} + \sum_{j,k}\frac{h^{(j)}-z}{(h^{(k)}-z)^2}\operatorname{tr}\{P^{(k)},P^{(j)},P^{(k)}\} \\
&= 2\sum_j \frac{1}{h^{(j)}-z}\operatorname{tr}\{P^{(j)},P^{(j)},P^{(j)}\} - 2\sum_{j,k}\frac{1}{h^{(k)}-z}\operatorname{tr}\{P^{(k)},P^{(j)},P^{(k)}\} \\
&\quad + \sum_{j,k}\frac{h^{(j)}-z}{(h^{(k)}-z)^2}\operatorname{tr}\{P^{(k)},P^{(j)},P^{(k)}\} \\
&= 2\sum_j \frac{1}{h^{(j)}-z}\operatorname{tr}\{P^{(j)},P^{(j)},P^{(j)}\} - 2\sum_{k}\frac{1}{h^{(k)}-z}\operatorname{tr}\{P^{(k)},P^{(k)}\} \\
&\quad + \sum_{j,k}\frac{1}{(h^{(k)}-z)^2}\operatorname{tr}\{P^{(k)},h^{(j)}P^{(j)},P^{(k)}\} - z\sum_k \frac{1}{(h^{(k)}-z)^2}\operatorname{tr}\{P^{(k)},P^{(k)}\} \\
&= 2\sum_j \frac{1}{h^{(j)}-z}\operatorname{tr}\{P^{(j)},P^{(j)},P^{(j)}\} + \sum_k \frac{1}{(h^{(k)}-z)^2}\operatorname{tr}\{P^{(k)},A_1,P^{(k)}\} \\
&= 2\sum_j \frac{1}{h^{(j)}-z}\operatorname{tr}\{P^{(j)},P^{(j)},P^{(j)}\} + \sum_j \frac{1}{(h^{(j)}-z)^2}\operatorname{tr}\{P^{(j)},A_1,P^{(j)}\} \\
&= 2\sum_j \frac{1}{h^{(j)}-z}\operatorname{tr}\{P^{(j)},P^{(j)},P^{(j)}\} + \sum_j \frac{1}{(h^{(j)}-z)^2}\operatorname{tr}\{P^{(j)},A_1-h^{(j)}I,P^{(j)}\},
\end{aligned} \tag{F.4}$$

where we used the identities $\sum_j P^{(j)} = I$, $\{P^{(k)},P^{(k)}\}=0$ and (3.3). Substituting (F.4) into (4.3), we arrive at (4.5).

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A Lieb–Thirring type inequality for magnetic Schrödinger operators with a radial symmetry

Diana Barseghyan and Françoise Truc

This paper is dedicated to Professor Boris Pavlov, a great scientist and a man of great humanity.

Abstract. The aim of the paper is to derive spectral estimates on the eigenvalue moments of the magnetic Schrödinger operators defined on the two-dimensional disk with a radially symmetric magnetic field and radially symmetric electric potential.

Keywords. Eigenvalue bounds, radial magnetic field, Lieb–Thirring inequalities, discrete spectrum.

1. Introduction

Let us consider a particle in a bounded domain Ω in $\mathbb{R}^2$ in the presence of a magnetic field B and an electric potential V. We define the 2-dimensional magnetic Schrödinger operator associated to this particle as follows:

Let A be a magnetic potential associated to B, i.e. a smooth real valued-function on $\Omega \subset \mathbb{R}^2$ verifying $\mathrm{rot}\,(A) = B$ and $V \geq 0$ be a bounded measurable potential defined on $L^2(\Omega)$. The magnetic Schrödinger operator is initially defined on $C_0^\infty(\Omega)$ by $H_\Omega(A,V) = (i\nabla + A)^2 - V$.

The case of a non-constant magnetic field can be motivated by anisotropic superconductors (see, for instance, [4]) or the liquid crystal theory.

Assuming some regularity conditions (RC) on A, namely, the magnetic field $B \in L^\infty_{\mathrm{loc}}(\Omega)$ and the corresponding magnetic potential $A \in L^\infty(\Omega)$, we get that the magnetic Sobolev norm $\|(i\nabla + A)u\|_{L^2(\Omega)},\ u \in \mathcal{H}_0^1(\Omega)$, is closed and equivalent to the non-magnetic one, which means that they both have purely discrete spectrum. Thus using the boundedness of the potential V the self-adjoint Friedrichs extension of $H_\Omega(A,V)$, initially defined on $C_0^\infty(\Omega)$, has a purely discrete spectrum.

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In the paper we also consider the case when the magnetic field grows to infinity as the variable approaches the boundary and has a non zero infimum

$$B(z) \to \infty \quad \text{as } z \to \partial\Omega \quad \text{and} \quad K := \inf B(z) > 0. \tag{1.1}$$

In view of the lower bound

$$(H_\Omega(A,V)(u),u)_{L^2(\Omega)} \geq \int_\Omega \left(B(z) - \|V\|_{L^\infty(\Omega)}\right) |u|^2(z)\,\mathrm{d}z,$$

one again can construct the Friedrichs extension of $H_\Omega(A,V)$ initially defined on $C_0^\infty(\Omega)$. Moreover, it still has a purely discrete spectrum [15].

For simplicity, we will use for the Friedrichs extension the same symbol $H_\Omega(A,V)$, and we shall denote the increasingly ordered sequence of its eigenvalues by $\lambda_k = \lambda_k(\Omega,A,V)$.

The purpose of this paper is to establish bounds of the eigenvalue moments of such operators. Let us recall the following bound which was proved by Berezin, Li and Yau for non-magnetic Dirichlet Laplacians on a domain Ω in $\mathbb{R}^d$; see [1, 2, 14],

$$\sum_k (\Lambda - \lambda_k(\Omega,0,0))_+^\sigma \leq L^{\mathrm{cl}}_{\sigma,d}\,|\Omega|\,\Lambda^{\sigma+\frac{d}{2}} \quad \text{for any } \sigma \geq 1 \text{ and } \Lambda > 0\,, \tag{1.2}$$

where $|\Omega|$ is the volume of Ω, and the constant on the right-hand side,

$$L^{\mathrm{cl}}_{\sigma,d} = \frac{\Gamma(\sigma+1)}{(4\pi)^{\frac{d}{2}}\Gamma(\sigma+1+d/2)}\,, \tag{1.3}$$

is optimal. Moreover, for $0 \leq \sigma < 1$, the bound (1.2) still exists, but with another constant on the right-hand side [10]

$$\sum_k (\Lambda - \lambda_k(\Omega,0,0))_+^\sigma \leq 2\left(\frac{\sigma}{\sigma+1}\right)^\sigma L^{\mathrm{cl}}_{\sigma,d}\,|\Omega|\,\Lambda^{\sigma+\frac{d}{2}}\,, \quad 0 \leq \sigma < 1\,. \tag{1.4}$$

For Schrödinger operators $H_\Omega(0,V)$ with Dirichlet boundary conditions the following bound was proved by Lieb–Thirring [12]:

$$\sum_{\lambda_k(\Omega,0,V)\leq 0} |\lambda_k(\Omega,0,V)|^\sigma \leq L^{\mathrm{cl}}_{\sigma,d}\int_\Omega V^{\sigma+d/2}(x)\,\mathrm{d}x\,, \quad \sigma \geq 3/2\,. \tag{1.5}$$

There exists a similar estimate for Schrödinger operators $H_\Omega(A,V)$ with Dirichlet boundary conditions and with non-zero magnetic field [13]

$$\sum_{\lambda_k(\Omega,A,V)\leq 0} |\lambda_k(\Omega,A,V)|^\sigma \leq L^{\mathrm{cl}}_{\sigma,d}\int_\Omega V^{\sigma+d/2}(x)\,\mathrm{d}x\,, \quad \sigma \geq 3/2\,. \tag{1.6}$$

In the magnetic case, due to the pointwise diamagnetic inequality, which means that under rather general assumptions on the magnetic potentials [11]

$$|\nabla|u(x)|| \leq |(i\nabla + A)u(x)| \quad \text{for a.a. } x \in \Omega\,,$$

we get that $\lambda_1(\Omega,A,0) \geq \lambda_1(\Omega,0,0)$. However, the estimate

$$\lambda_j(\Omega,A,0) \geq \lambda_j(\Omega,0,0)$$

fails in general if $j \geq 2$. We remark that, nevertheless, momentum estimates are still valid for some values of the parameters. In particular, it was shown [13] that the sharp bound (1.2) holds true for arbitrary magnetic fields provided $\sigma \geq 3/2$, and for constant magnetic fields if $\sigma \geq 1$ [7, 9]. In the two-dimensional case the bound (1.4) holds true for constant magnetic fields if $0 \leq \sigma < 1$, and the constant on the right-hand side cannot be improved [8].

In the present work we study the magnetic Schrödinger operators $H_\Omega(A, V)$ defined on the two- dimensional disk Ω centered in zero and with radius $r_0 > 0$, with a radially symmetric magnetic field $B(x) = B(|x|)$ and electric potential $V = V(|x|) \geq 0$. Our aim is to extend a sufficiently precise Lieb–Thirring type inequality to this situation. A similar problem was studied recently for magnetic Dirichlet Laplacians in [3], but under very strong restrictions on the growth of the magnetic field.

Let us also mention that some estimates on the counting function of the eigenvalues of the magnetic Dirichlet Laplacian on a disk were established in [15], in the case where the field is radial and satisfies some growth condition near the boundary.

2. Main Result

Inspired by the weighted one-dimensional Lieb–Thirring type inequalities [6] we establish the weighted eigenvalue bound for the operator $H_\Omega(A, V)$ in terms of the magnetic and electric potentials B and V. The following theorem holds true:

Theorem 2.1. *Let $H_\Omega(A, V)$ be a magnetic Schrödinger operator with Dirichlet boundary conditions defined on the disk Ω of radius r_0 centered in zero with a radial magnetic field $B(x) = B(|x|)$ and an electric potential $V = V(|x|) \geq 0$. Let us assume the validity of the conditions (RC) or the validity of* (1.1). *Then for any $0 < \varepsilon \leq 3/4$, $0 \leq \alpha < 1$ and $\sigma \geq (1-\alpha)/2$, the following inequality holds:*

$$
\begin{aligned}
&\operatorname{tr}\left(H_\Omega(A, V)\right)_-^\sigma \\
&\leq \frac{2r_0 L_{\sigma+1/2,\alpha}}{\sqrt{1-\varepsilon}} \int_0^{r_0} \left(\left(\frac{1}{\varepsilon} - 1\right) \frac{1}{r^2} \left(\int_0^r sB(s)\,\mathrm{d}s \right)^2 + V(r) - \frac{1}{4r^2} \right)_+^{\sigma+1+\alpha/2} r^\alpha\,\mathrm{d}r \\
&\quad + \frac{L_{\sigma,\alpha}}{\sqrt{1-\varepsilon}} \int_0^{r_0} \left(\left(\frac{1}{\varepsilon} - 1\right) \frac{1}{r^2} \left(\int_0^r sB(s)\,\mathrm{d}s \right)^2 + V(r) - \frac{1}{4r^2} \right)_+^{\sigma+(1+\alpha)/2} r^\alpha\,\mathrm{d}r \\
&\quad + L_{\sigma,\alpha} \int_0^{r_0} \left(V(r) - \frac{1}{r^2} \left(\int_0^r sB(s)\,\mathrm{d}s \right)^2 \right)_+^{\sigma+(1+\alpha)/2} r^\alpha\,\mathrm{d}r,
\end{aligned} \tag{2.1}
$$

where $L_{\sigma+1/2,\alpha}$ and $L_{\sigma,\alpha}$ are some constants.

Remark 2.1. If $0 \le \sigma < 3/2$ then, even for magnetic Laplacians, (1.2)-type inequality is known only for constant magnetic fields.

Remark 2.2. If

$$\sup_{r<r_0}\left(V(r)-\frac{1}{4r^2}\right) < -A^2/3,$$

where

$$A=\sup_{r<r_0}\frac{1}{r}\int_0^r sB(s)\mathrm{d}s<\infty$$

then we can choose $\varepsilon \ge 3/4$ such that the first two terms of the right-hand side of (2.1) be equal to zero. So we decrease the order of the potential V in Lieb–Thirring bound (1.6) from $\sigma+1$ to $\sigma+(1+\alpha)/2<\sigma+1$.

Proof. We begin by recalling the standard partial wave decomposition [5]:

$$L^2(\Omega,dx)=\bigoplus_{m=-\infty}^{\infty} L^2((0,r_0),2\pi r dr)$$

$$f\to(\dots,f_{-1},f_0,f_1,\dots)\quad\text{with } f(r,\theta)=\sum_{m=-\infty}^{\infty} e^{im\theta}f_m(r)\ .$$

Choosing the radial gauge $A(r,\theta)=(-a(r)\sin\theta, a(r)\cos\theta)$ where

$$a(r):=\frac{1}{r}\int_0^r sB(s)\,\mathrm{d}s,$$

we get that the operator $H_\Omega(A,V)$ acts on $\bigoplus_{m=-\infty}^{\infty} L^2(0,r_0)$ as follows:

$$H_\Omega(A,V)=\bigoplus_{m=-\infty}^{\infty} h_m(B,V),$$

where the operators $h_m(B,V)$ are the Friedrichs extension of the closures of the quadratic forms

$$Q(h_m(B,V))[u]=2\pi\int_0^{r_0}\left(\left|\frac{\mathrm{d}u}{\mathrm{d}r}\right|^2+\left(\frac{m}{r}-a(r)\,\mathrm{d}s\right)^2|u|^2-V|u|^2\right) r\,\mathrm{d}r,$$

defined originally on $C_0^\infty(0,r_0)$, and acting on their domain as

$$h_m(B,V)=-\frac{\mathrm{d}^2}{\mathrm{d}r^2}-\frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}r}+\left(\frac{m}{r}-a(r)\right)^2-V(r).$$

Employing the mapping $U: C_0^\infty(0,r_0)\to C_0^\infty(0,r_0)$ defined by

$$(Uf)(r)=\frac{1}{\sqrt{2\pi r}}f(r),$$

one gets the unitarily equivalence between the operators $h_m(B,V)$ and

$$l_m(B,V)=-\frac{\mathrm{d}^2}{\mathrm{d}r^2}-\frac{1}{4r^2}+\left(\frac{m}{r}-a(r)\right)^2-V(r)$$

defined already on $L^2((0,r_0),dr)$. Thus we are going to consider the self-adjoint operators associated to the closures of the quadratic forms

$$Q(l_m(B,V))[v] = \int_0^{r_0} \left(\left|\frac{\mathrm{d}v}{\mathrm{d}r}\right|^2 - \frac{1}{4r^2}|v|^2 + \left(\frac{m}{r} - a(r)\right)^2 |v|^2 - V(r)|v|^2 \right) \mathrm{d}r,$$

defined originally on $C_0^\infty(0,r_0)$.

We have, for any $0<\varepsilon<1$ and any $v \in C_0^\infty(0,r_0)$,

$$\begin{aligned} &Q(l_m(B,V))[v] \\ &= \int_0^{r_0} \left(\left|\frac{\mathrm{d}v}{\mathrm{d}r}\right|^2 - \frac{1}{4r^2}|v|^2 + \frac{m^2}{r^2}|v|^2 - \frac{2m}{r}a(r)|v|^2 + a^2(r)|v|^2 - V(r)|v|^2 \right) \mathrm{d}r \\ &\geq \int_0^{r_0} \left(\left|\frac{\mathrm{d}v}{\mathrm{d}r}\right|^2 - \frac{1}{4r^2}|v|^2 + \frac{m^2}{r^2}|v|^2 - \frac{m^2\varepsilon}{r^2}|v|^2 \right. \\ &\qquad \left. - \frac{1}{\varepsilon}a^2(r)|v|^2 + a^2(r)|v|^2 - V(r)|v|^2 \right) \mathrm{d}r. \end{aligned}$$

It follows from the above inequality that if $m \neq 0$ and $0<\varepsilon \leq 3/4$, then

$$l_m(B,V) \geq g_{B,V} + \frac{(1-\varepsilon)m^2 - 1/4}{r_0^2}, \tag{2.2}$$

where the operator $g_{B,V}$ is associated with the closure of the form

$$Q(g_{B,V})[v] = \int_0^{r_0} \left(\left|\frac{\mathrm{d}v}{\mathrm{d}r}\right|^2 - \left(\frac{1}{\varepsilon} - 1\right) a^2(r)|v|^2 - V(r)|v|^2 \right) \mathrm{d}r$$

initially defined on $C_0^\infty(0,r_0)$.

Let $\{\mu_k(B,V)\}_{k=1}^{\infty}$ be the set of the negative eigenvalues of $g_{B,V}$. Due to the minimax principle, inequality (2.2) implies

$$
\begin{aligned}
&\operatorname{tr}\left(\bigoplus_{m=-\infty}^{\infty} h_m(B,V)\right)_-^{\sigma}\\
&\le \sum_{\substack{m=-\infty\\ m\neq 0}}^{\infty} \operatorname{tr}\left(g_{B,V}+\frac{(1-\varepsilon)m^2-1/4}{r_0^2}\right)_-^{\sigma} + \operatorname{tr}\left(-\frac{\mathrm{d}^2}{\mathrm{d}r^2}-\frac{1}{4r^2}+a^2(r)-V(r)\right)_-^{\sigma}\\
&\le \sum_{\substack{m=-\infty\\ m\neq 0}}^{\infty} \sum_{\mu_k(B,V)+((1-\varepsilon)m^2-1/4)/r_0^2\le 0} \left|\mu_k(B,V)+\frac{(1-\varepsilon)m^2-1/4}{r_0^2}\right|^{\sigma}\\
&\quad + \operatorname{tr}\left(-\frac{\mathrm{d}^2}{\mathrm{d}r^2}-\frac{1}{4r^2}+a^2(r)-V(r)\right)_-^{\sigma}\\
&\le \sum_{k=1}^{\infty} \sum_{0<|m|\le\sqrt{\frac{|\mu_k(B,V)|r_0^2+1/4}{1-\varepsilon}}} \left|\mu_k(B,V)+\frac{(1-\varepsilon)m^2-1/4}{r_0^2}\right|^{\sigma}\\
&\quad + \operatorname{tr}\left(-\frac{\mathrm{d}^2}{\mathrm{d}r^2}-\frac{1}{4r^2}+a^2(r)-V(r)\right)_-^{\sigma}\\
&\le \sum_{k=1}^{\infty}\left(\frac{2\sqrt{|\mu_k(B,V)|r_0^2+1/4}}{\sqrt{1-\varepsilon}}|\mu_k(B,V)|^{\sigma}\right)\\
&\quad + \operatorname{tr}\left(-\frac{\mathrm{d}^2}{\mathrm{d}r^2}-\frac{1}{4r^2}+a^2(r)-V(r)\right)_-^{\sigma}\\
&\le \frac{2r_0}{\sqrt{1-\varepsilon}}\sum_{k=1}^{\infty}|\mu_k(B,V)|^{\sigma+1/2} + \frac{1}{\sqrt{1-\varepsilon}}\sum_{k=1}^{\infty}|\mu_k(B,V)|^{\sigma}\\
&\quad + \operatorname{tr}\left(-\frac{\mathrm{d}^2}{\mathrm{d}r^2}-\frac{1}{4r^2}+a^2(r)-V(r)\right)_-^{\sigma}.
\end{aligned}
\tag{2.3}
$$

Let us extend the potential $-\left(\frac{1}{\varepsilon}-1\right)a^2(r)-V(r)$ to $\mathbb{R}_+$ by zero and denote the corresponding one-dimensional Schrödinger operator by $g^*(B,V)$. Since

$$C_0^{\infty}(0,r_0)\subset C_0^{\infty}(\mathbb{R}_+),$$

by minimax principle for any $\delta>0$,

$$\sum_k |\mu_k(B,V)|^{\delta} \le \sum_k |\nu_k(B,V)|^{\delta}, \tag{2.4}$$

where $\{\nu_k(B,V)\}_{k=1}^{\infty}$ are the negative eigenvalues of $g^*(B,V)$.

Applying the Lieb–Thirring inequality [6], for any $\alpha \in [0,1)$ and $\sigma \geq (1-\alpha)/2$, we get

$$\sum_{k=1}^{\infty} |\nu_k(B,V)|^{\sigma+1/2} \leq L_{\sigma+1/2,\alpha} \int_0^{r_0} \left(\left[\frac{1}{\varepsilon}-1\right] a^2(r) + V(r) - \frac{1}{4r^2}\right)_+^{\sigma+1+\alpha/2} r^{\alpha}\, \mathrm{d}r,$$

$$\sum_{k=1}^{\infty} |\nu_k(B,V)|^{\sigma} \leq L_{\sigma,\alpha} \int_0^{r_0} \left(\left[\frac{1}{\varepsilon}-1\right] a^2(r) + V(r) - \frac{1}{4r^2}\right)_+^{\sigma+(1+\alpha)/2} r^{\alpha}\, \mathrm{d}r, \quad (2.5)$$

$$\operatorname{tr}\left(-\frac{\mathrm{d}^2}{\mathrm{d}r^2} - \frac{1}{4r^2} + a^2(r) - V(r)\right)_-^{\sigma} \leq L_{\sigma,\alpha} \int_0^{r_0} \left(V(r) - a^2(r)\right)_+^{\sigma+(1+\alpha)/2} r^{\alpha}\, \mathrm{d}r.$$

where $L_{\sigma+1/2,\alpha}$ and $L_{\sigma,\alpha}$ are some constants.

This, together with the estimates (2.3)–(2.4), means

$$\begin{aligned} &\operatorname{tr}\left(\bigoplus_{m=-\infty}^{\infty} h_m(B,V)\right)_-^{\sigma} \\ &\leq \frac{2r_0 L_{\sigma+1/2,\alpha}}{\sqrt{1-\varepsilon}} \int_0^{r_0} \left(\left(\frac{1}{\varepsilon}-1\right) a^2(r) + V(r) - \frac{1}{4r^2}\right)_+^{\sigma+1+\alpha/2} r^{\alpha}\, \mathrm{d}r \\ &\quad + \frac{L_{\sigma,\alpha}}{\sqrt{1-\varepsilon}} \int_0^{r_0} \left(\left(\frac{1}{\varepsilon}-1\right) a^2(r) + V(r) - \frac{1}{4r^2}\right)_+^{\sigma+(1+\alpha)/2} r^{\alpha}\, \mathrm{d}r \\ &\quad + L_{\sigma,\alpha} \int_0^{r_0} \left(V(r) - a^2(r)\right)_+^{\sigma+(1+\alpha)/2} r^{\alpha}\, \mathrm{d}r, \end{aligned} \quad (2.6)$$

which proves the theorem. □

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Scattering matrices and Weyl functions of quasi boundary triples

Jussi Behrndt and Hagen Neidhardt

In memory of Boris Sergeevich Pavlov

Abstract. In this note a representation formula for the scattering matrix of a pair of self-adjoint extensions of a non-densely defined symmetric operator with infinite deficiency indices is proved with the help of quasi boundary triples and their Weyl functions. This result is a generalization of a classical formula by V.A. Adamyan and B.S. Pavlov.

1. Introduction

Mathematical scattering theory and its applications is a central theme in the works of B.S. Pavlov. Among his numerous contributions in this area we mention here the works [1, 3, 4, 5, 8, 26, 36, 37, 39, 40, 41, 42, 43] and we point out the famous classical paper [2], which can also be viewed as the origin of the present note on scattering matrices. In fact, in [2] V.A. Adamyan and B.S. Pavlov proved a representation formula in terms of M.G. Krein's Q-function for the scattering matrix of a pair of self-adjoint extensions A and B of a symmetric operator with finite deficiency indices (see also [6]). In this situation the resolvents of A and B differ by a finite rank operator, that is,

$$\dim\big(\operatorname{ran}\big((A-\lambda)^{-1}-(B-\lambda)^{-1}\big)\big)<\infty \tag{1.1}$$

holds for some (and hence for all) $\lambda \in \rho(A)\cap\rho(B)$, and the S-matrix becomes a matrix-valued function in a spectral representation of the absolutely continuous part of A. This important result was revisited and newly interpreted in [15] using the concept of ordinary boundary triples and their Weyl functions from extension theory of symmetric operators, see also [14, 16]. Only very recently in [17] the finite rank condition (1.1) was relaxed and, roughly speaking, replaced by the typical trace class assumption

$$(A-\lambda)^{-1}-(B-\lambda)^{-1}\in\mathfrak{S}_1 \tag{1.2}$$

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for some (and hence for all) $\lambda \in \rho(A) \cap \rho(B)$. In this more general situation it is convenient to work with so-called generalized or quasi boundary triples, instead of ordinary boundary triples, in particular, this allows to apply the representation formula for the S-matrix to scattering problems involving different self-adjoint realizations of second order elliptic PDEs on unbounded domains. For related recent results we also refer the reader to [33, 34, 35].

The main objective of the present note on scattering matrices is to provide a slight generalization of the main representation formula for the scattering matrix in [17]. Here we shall extend [17, Theorem 3.1] in two directions. Firstly, we formulate and prove the representation formula in the framework of quasi boundary triples (instead of generalized boundary triples), which allows a bit more flexibility in applications to differential operators (see also [10, 17]), and secondly, we drop the assumption that the underlying symmetric operator is densely defined. We also note that the trace class condition (1.2) will follow automatically from our assumptions on the γ-field and Weyl function M of the quasi boundary triple; instead of $\mathfrak{S}_1$-regularity of the Weyl function as in [17, Theorem 3.1] we shall impose a Hilbert–Schmidt condition on the γ-field and require the values of M^{-1} to be bounded. The present generalizations lead to some technical difficulties in the proof of the representation formula for the S-matrix. More precisely, since the values of the Weyl function of a quasi boundary triple may be non-closed and unbounded operators, particular attention has to be paid in some of the main steps of the proof. Furthermore, if the domain of the underlying symmetric operator is not dense the adjoint needs to be interpreted in the sense of linear relations (multi-valued operators) and hence it is necessary to use boundary triple techniques for linear relations here. However, these additional efforts are worthwhile since problems in mathematical scattering theory naturally lead to non-densely defined symmetric defined operators. As an example we consider a scattering system consisting of one-dimensional Schrödinger operators with a real-valued bounded integrable potential in $L^2(\mathbb{R})$. Here the underlying symmetric operator is defined on all $H^2(\mathbb{R})$-functions that vanish on the support of the potential, and hence is non-densely defined. We shall illustrate how a quasi boundary triple for the adjoint relation can be chosen and derive a representation of the scattering matrix in this case from our main result Theorem 3.1.

2. Scattering systems and Weyl functions of quasi boundary triples

Let A and B be self-adjoint operators in a separable Hilbert space $\mathfrak{H}$. The pair $\{A, B\}$ may be viewed as a scattering system, where A stands for the unperturbed operator and B for the perturbed operator. In this preparatory section we do not impose any conditions on the type of the perturbation. We shall discuss in the following how (quasi) boundary triples may be used to regard A and B as self-adjoint extensions of an underlying symmetric operator and how the resolvent difference of A and B can be factorized in a convenient Krein type formula. In the following operators will often be identified with their graphs.

Let $S = A \cap B$ be the intersection (of the graphs) of A and B. Then S is given by

$$Sf := Af = Bf, \quad \operatorname{dom} S = \bigl\{f \in \operatorname{dom} A \cap \operatorname{dom} B : Af = Bf\bigr\}. \tag{2.1}$$

In general the domain of S is not a dense subspace of $\mathfrak{H}$, and it may happen that $\operatorname{dom} S = \{0\}$. However, S is a closed operator in $\mathfrak{H}$ and since A and B are self-adjoint extensions of S it is clear that S is a symmetric operator in $\mathfrak{H}$. The adjoint S^* of S is defined as the linear relation

$$S^* = \bigl\{\{g, g'\} : (Sf, g) = (f, g') \text{ for all } f \in \operatorname{dom} S\bigr\} \subset \mathfrak{H} \times \mathfrak{H};$$

here and in the following we write elements in linear relations (linear subspaces) in a pair notation, e.g., $\{g, g'\}$. It is clear that S^* is (the graph of) an operator if and only if $\operatorname{dom} S$ is dense in $\mathfrak{H}$, otherwise S^* has a nontrivial multivalued part (that is, there exists elements of the form $\{0, g'\} \in S^*$, $g' \neq 0$). We shall view A and B as self-adjoint restrictions of the adjoint relation S^* and use the techniques of (quasi) boundary triples from extension theory of symmetric operators and relations. We refer the reader to [7, 24, 25, 27] for more details on linear relations and to [11, 12, 20, 21, 22, 23, 29, 46] for the notion of ordinary, generalized, and quasi boundary triples for linear operators and relations. In the following we repeat a few necessary definitions from [11, 12] and provide a useful factorization of the difference of the resolvents of A and B in Proposition 2.4.

Definition 2.1. *Let T be a linear relation in the Hilbert space $\mathfrak{H}$ such that $\overline{T} = S^*$. Then $\Pi = \{\mathcal{G}, \Gamma_0, \Gamma_1\}$ is said to be a quasi boundary triple for S^* if $\mathcal{G}$ is a Hilbert space and $\Gamma_0, \Gamma_1 : T \to \mathcal{G}$ are linear mappings such that the following conditions* (i)–(iii) *are satisfied.*

(i) *The abstract Green's identity*

$$(f', g) - (f, g') = (\Gamma_1 \widehat{f}, \Gamma_0 \widehat{g}) - (\Gamma_0 \widehat{f}, \Gamma_1 \widehat{g})$$

holds for all $\widehat{f} = \{f, f'\}$, $\widehat{g} = \{g, g'\} \in T$;

(ii) *The range of the mapping $(\Gamma_0, \Gamma_1)^\top : T \to \mathcal{G} \times \mathcal{G}$ is dense;*

(iii) *$A_0 := \ker \Gamma_0$ is a self-adjoint relation in $\mathfrak{H}$.*

Assume that $\Pi = \{\mathcal{G}, \Gamma_0, \Gamma_1\}$ is a quasi boundary triple for $\overline{T} = S^*$ and let $A_0 = \ker \Gamma_0$. For $\lambda \in \rho(A_0)$ one verifies the direct sum decomposition

$$T = A_0 \,\widehat{+}\, \widehat{\mathcal{N}}_\lambda(T), \quad \widehat{\mathcal{N}}_\lambda(T) = \bigl\{\{f_\lambda, \lambda f_\lambda\} : f_\lambda \in \ker(T - \lambda)\bigr\}, \tag{2.2}$$

which implies that $\Gamma_0 \upharpoonright \widehat{\mathcal{N}}_\lambda(T)$ is invertible. In the decomposition (2.2) the direct sum $\mathcal{A} \widehat{+} \mathcal{N}$ of linear relations $\mathcal{A}$ and $\mathcal{N}$ such that $\mathcal{A} \cap \mathcal{N} = \{0\}$ is defined by $\mathcal{A} \widehat{+} \mathcal{N} = \{f + g, f' + g'\}$, where $\{f, f'\} \in \mathcal{A}$ and $\{g, g'\} \in \mathcal{N}$.

We then define the γ-field and Weyl function corresponding to the quasi boundary triple $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ as operator functions on $\rho(A_0)$ by

$$\lambda \mapsto \gamma(\lambda) = \pi_1 \bigl(\Gamma_0 \upharpoonright \widehat{\mathcal{N}}_\lambda(T)\bigr)^{-1} \quad \text{and} \quad \lambda \mapsto M(\lambda) = \Gamma_1 \bigl(\Gamma_0 \upharpoonright \widehat{\mathcal{N}}_\lambda(T)\bigr)^{-1};$$

here π_1 denotes the projection onto the first component of $\mathfrak{H} \times \mathfrak{H}$. We refer the reader to [11, 12] for a detailed discussion of the properties of the γ-field and Weyl function; here we only recall [11, Proposition 2.6].

Proposition 2.2. *Let $\Pi = \{\mathcal{G}, \Gamma_0, \Gamma_1\}$ be a quasi boundary triple for S^* with γ-field γ and Weyl function M. For $\lambda, \mu \in \rho(A_0)$ the following holds.*

(i) *$\gamma(\lambda)$ is a densely defined operator from $\mathcal{G}$ into $\mathfrak{H}$ with $\operatorname{dom}\gamma(\lambda) = \operatorname{ran}\Gamma_0$ such that the function $\lambda \mapsto \gamma(\lambda)\varphi$ is holomorphic on $\rho(A_0)$ for every $\varphi \in \operatorname{ran}\Gamma_0$ and*
$$\gamma(\lambda) = \big(I + (\lambda - \mu)(A_0 - \lambda)^{-1}\big)\gamma(\mu)$$
holds. Moreover, for each $\lambda \in \rho(A_0)$ the operator $\gamma(\lambda)$ is closable and its closure $\overline{\gamma(\lambda)}$ is a bounded operator from $\mathcal{G}$ into $\mathfrak{H}$.

(ii) *$\gamma(\overline{\lambda})^*$ is a bounded mapping defined on $\mathfrak{H}$ with values in $\operatorname{ran}\Gamma_1 \subset \mathcal{G}$ and for all $h \in \mathfrak{H}$ we have*
$$\gamma(\overline{\lambda})^* h = \Gamma_1 \begin{pmatrix} (A_0 - \lambda)^{-1} h \\ (I + \lambda(A_0 - \lambda)^{-1})h \end{pmatrix}.$$

(iii) *$M(\lambda)$ is a densely defined operator in $\mathcal{G}$ with*
$$\operatorname{dom} M(\lambda) = \operatorname{ran}\Gamma_0 \text{ and } \operatorname{ran} M(\lambda) \subset \operatorname{ran}\Gamma_1.$$

(iv) *$M(\lambda)\Gamma_0 \widehat{f}_\lambda = \Gamma_1 \widehat{f}_\lambda$ for all $\widehat{f}_\lambda \in \widehat{\mathcal{N}}_\lambda(T)$.*

(v) *$M(\lambda) \subseteq M(\overline{\lambda})^*$ and*
$$M(\lambda)\varphi - M(\mu)^*\varphi = (\lambda - \overline{\mu})\gamma(\mu)^*\gamma(\lambda)\varphi, \quad \varphi \in \operatorname{dom} M(\lambda).$$
The function $\lambda \mapsto M(\lambda)$ is holomorphic in the sense that it can be written as $M(\lambda) = C + L(\lambda)$, where
$$C\varphi := \operatorname{Re} M(i)\varphi = \frac{1}{2}(M(i) + M(i)^*)\varphi, \quad \varphi \in \operatorname{dom} C := \operatorname{dom} M(i),$$
is a possible unbounded symmetric operator and $L(\lambda)$ is given by
$$L(\lambda) := \gamma(i)^*(\lambda + (1 + \lambda^2)(A_0 - \lambda)^{-1})\overline{\gamma(i)}, \quad \lambda \in \rho(A_0).$$

In the next lemma we show that the inclusion $\operatorname{ran} M(\lambda) \subset \operatorname{ran}\Gamma_1$ in Proposition 2.2 (iii) becomes an equality if the relation $A_1 := \ker\Gamma_1$ is assumed to be self-adjoint in $\mathfrak{H}$. Note that by Green's identity A_1 is automatically symmetric.

Lemma 2.3. *Let $\Pi = \{\mathcal{G}, \Gamma_0, \Gamma_1\}$ be a quasi boundary triple for S^* with Weyl function M and assume, in addition, that $A_1 = \ker\Gamma_1$ is a self-adjoint relation in $\mathfrak{H}$. Then for all $\lambda \in \rho(A_0) \cap \rho(A_1)$ the operator $M(\lambda)$ maps $\operatorname{ran}\Gamma_0$ onto $\operatorname{ran}\Gamma_1$ and $M(\lambda)^{-1}$ exist and is defined on $\operatorname{ran}\Gamma_1$.*

Proof. The assumption that $A_1 = \ker\Gamma_1$ is self-adjoint implies that the transposed triple $\Pi^\top = \{\mathcal{G}, \Gamma_1, -\Gamma_0\}$ is also quasi boundary triple for S^*. The corresponding Weyl function $M^\top(\lambda)$, $\lambda \in \rho(A_1)$, is defined on $\operatorname{ran}\Gamma_1$ and has values in $\operatorname{ran}\Gamma_0$. One easily checks that $M^\top(\lambda)M(\lambda)g = -g$, $g \in \operatorname{ran}\Gamma_0$, and $M(\lambda)M^\top(\lambda)h = -h$, $h \in \operatorname{ran}\Gamma_1$, $\lambda \in \rho(A_0) \cap \rho(A_1)$. Hence $M(\lambda)$ maps $\operatorname{ran}\Gamma_0$ onto $\operatorname{ran}\Gamma_1$ and is invertible. □

The next result will be used in the formulation and proof of our abstract representation formula for the scattering matrix in the next section. The statement on the existence of a quasi boundary triple follows for the case that S is densely defined also from [17, Proposition 2.9 (i)] and the Krein-type resolvent formula in (2.4) is a special case of [12, Corollary 6.17] or [13, Corollary 3.9].

Proposition 2.4. *Let A and B be self-adjoint operators in $\mathfrak{H}$ and consider the closed symmetric operator $S = A \cap B$. Then the closure of the linear relation $T = A \widehat{+} B$ coincides with the adjoint relation S^* and there exists a quasi boundary triple $\Pi = \{\mathcal{G}, \Gamma_0, \Gamma_1\}$ for $T \subset S^*$ such that*

$$A = \ker \Gamma_0 \quad \textit{and} \quad B = \ker \Gamma_1. \tag{2.3}$$

Furthermore, if γ and M are the corresponding γ-field and Weyl function then

$$(B-\lambda)^{-1} - (A-\lambda)^{-1} = -\gamma(\lambda)M(\lambda)^{-1}\gamma(\overline{\lambda})^*, \quad \lambda \in \rho(A) \cap \rho(B). \tag{2.4}$$

Proof. Since A and B are self-adjoint extensions of the closed symmetric operator $S = A \cap B$ (see also (2.1)) there exists an ordinary boundary triple $\Pi' = \{\mathcal{G}, \Lambda_0, \Lambda_1\}$ for S^* and a self-adjoint operator Θ in $\mathcal{G}$ such that

$$A = \ker \Lambda_0 \text{ and } B = \ker(\Lambda_1 - \Theta\Lambda_0). \tag{2.5}$$

We note that in the present situation the self-adjoint parameter Θ in $\mathcal{G}$ is an operator (and not a linear relation) since $S = A \cap B$, that is, A and B are disjoint self-adjoint extensions of S (cf. [20, 22, 23, 29]). Now consider the restriction $T := A \widehat{+} B$ of S^*. Since A and B are disjoint self-adjoint extensions of S it follows that $\overline{T} = S^*$, see [17, Proposition 2.9]. We claim that $\Pi = \{\mathcal{G}, \Gamma_0, \Gamma_1\}$, where

$$\Gamma_0 \widehat{f} := \Lambda_0 \widehat{f} \text{ and } \Gamma_1 \widehat{f} := \Lambda_1 \widehat{f} - \Theta\Lambda_0 \widehat{f}, \quad \widehat{f} \in T,$$

is a quasi boundary triple for $T \subset S^*$ such that (2.3) holds. In fact, (2.3) is clear from (2.5) and the definition of Γ_0 and Γ_1, and hence it remains to check items (i)–(iii) in Definition 2.1. For $\widehat{f} = \{f, f'\}, \widehat{g} = \{g, g'\} \in T$ one computes

$$\begin{aligned}(\Gamma_1\widehat{f}, \Gamma_0\widehat{g}) - (\Gamma_0\widehat{f}, \Gamma_1\widehat{g}) &= \bigl(\Lambda_1\widehat{f} - \Theta\Lambda_0\widehat{f}, \Lambda_0\widehat{g}\bigr) - \bigl(\Lambda_0\widehat{f}, \Lambda_1\widehat{g} - \Theta\Lambda_0\widehat{g}\bigr)\\ &= (\Lambda_1\widehat{f}, \Lambda_0\widehat{g}) - (\Lambda_0\widehat{f}, \Lambda_1\widehat{g})\\ &= (f', g) - (f, g')\end{aligned}$$

and hence the abstract Green's identity is valid. Next, assume that

$$0 = \left(\begin{pmatrix} \varphi \\ \psi \end{pmatrix}, \begin{pmatrix} \Gamma_0\widehat{f} \\ \Gamma_1\widehat{f} \end{pmatrix} \right) = \bigl(\varphi, \Lambda_0\widehat{f}\bigr) + \bigl(\psi, \Lambda_1\widehat{f} - \Theta\Lambda_0\widehat{f}\bigr)$$

holds for some $\varphi, \psi \in \mathcal{G}$ and all $\widehat{f} \in T$. Since $\Pi' = \{\mathcal{G}, \Lambda_0, \Lambda_1\}$ is an ordinary boundary triple the map $(\Lambda_0, \Lambda_1)^\top : S^* \to \mathcal{G} \times \mathcal{G}$ is surjective. It follows that $\Lambda_1 \upharpoonright \ker \Lambda_0$ maps onto $\mathcal{G}$ and hence for $\widehat{f} \in A = \ker \Lambda_0$ one has $0 = (\psi, \Lambda_1\widehat{f})$, and therefore, $\psi = 0$. Now $(\varphi, \Lambda_0\widehat{f}) = 0$ for $\widehat{f} \in T$, and the fact that the range of the restriction of Λ_0 onto T is dense in $\mathcal{G}$ (since $\Lambda_0 : S^* \to \mathcal{G}$ is surjective, continuous with respect to the norm on $S^* \subset \mathfrak{H} \times \mathfrak{H}$ and T is dense in S^*), yield $\varphi = 0$.

Therefore, the range of the mapping $(\Gamma_0, \Gamma_1)^\top : T \to \mathcal{G} \times \mathcal{G}$ is dense and hence condition (ii) in Definition 2.1 holds. Condition (iii) is clear from (2.3). Thus, we have shown that $\Pi = \{\mathcal{G}, \Gamma_0, \Gamma_1\}$ is a quasi boundary triple for $\overline{T} = S^*$.

Next, we verify the Krein-type resolvent formula (2.4). To this end we note that the right-hand side of (2.3) makes sense by Proposition 2.2 and Lemma 2.3. It remains to show the equality of the left- and right-hand sides. Let $g \in \mathfrak{H}$ and define $\widehat{f} = \{f, f'\} \in T = A_0 \widehat{+} \widehat{\mathcal{N}}_\lambda(T)$ by

$$\begin{aligned} f &:= (A-\lambda)^{-1} g - \gamma(\lambda) M(\lambda)^{-1} \gamma(\overline{\lambda})^* g, \\ f' &:= (1 + \lambda(A-\lambda)^{-1}) g - \lambda\gamma(\lambda) M(\lambda)^{-1} \gamma(\overline{\lambda})^* g. \end{aligned} \tag{2.6}$$

Proposition 2.2 (ii) and the definition of the Weyl function yield

$$\Gamma_1 \widehat{f} = \Gamma_1 \bigl\{ (A-\lambda)^{-1} g, (1+\lambda(A-\lambda)^{-1}) g \bigr\} - M(\lambda) M(\lambda)^{-1} \gamma(\overline{\lambda})^* g = 0$$

and hence $\widehat{f} \in \ker \Gamma_1 = B$. From (2.6), $A, B \subset T$, and $\operatorname{ran} \gamma(\lambda) = \ker(T-\lambda)$ one infers

$$(B-\lambda) f = (T-\lambda)(A-\lambda)^{-1} g - (T-\lambda)\gamma(\lambda) M(\lambda)^{-1} \gamma(\overline{\lambda})^* g = g$$

and together with (2.6) this yields the resolvent formula (2.4). □

3. Main result

Let again A and B be self-adjoint operators in a separable Hilbert space $\mathfrak{H}$, and assume first that

$$(B-\lambda)^{-1} - (A-\lambda)^{-1} \in \mathfrak{S}_1(\mathfrak{H}) \tag{3.1}$$

holds for some, and hence for all, $\lambda \in \rho(A) \cap \rho(B)$. Here the symbol $\mathfrak{S}_1$ is used for the ideal of trace class operators. The ideal of Hilbert–Schmidt operators will be denoted in a similar way by $\mathfrak{S}_2$. The trace class condition (3.1) will follow in Theorem 3.1 and Theorem 3.2 from other assumptions automatically. Denote the absolutely continuous subspaces of A and B by $\mathfrak{H}^{ac}(A)$ and $\mathfrak{H}^{ac}(B)$, respectively, let $P^{ac}(A)$ be the orthogonal projection onto $\mathfrak{H}^{ac}(A)$ and let

$$A^{ac} = A \upharpoonright (\operatorname{dom} A \cap \mathfrak{H}^{ac}(A))$$

be the absolutely continuous part of A. It is well known (see, e.g., [9, 32, 45, 48, 49]) that under the trace class condition (3.1) the wave operators

$$W_\pm(B, A) := s - \lim_{t \to \pm\infty} e^{itB} e^{-itA} P^{ac}(A)$$

exist and are complete, i.e., $\operatorname{ran}(W_\pm(B,A)) = \mathfrak{H}^{ac}(B)$. The scattering operator is defined as $S(A,B) := W_+(B,A)^* W_-(B,A)$ and it follows that $S(A,B)$ is a unitary operator in $\mathfrak{H}^{ac}(A)$. In the following we discuss a representation formula for the scattering matrix $\{S_{AB}(\lambda)\}_{\lambda \in \mathbb{R}}$, a family of unitary operators in a spectral representation of the absolutely continuous part A^{ac} of A (see, e.g., [9, Chap. 4]), which is unitarily equivalent to the scattering operator $S(A,B)$.

The next theorem is a generalization of [17, Theorem 3.1] (see also [15, Theorem 3.8]). Instead of generalized boundary triples the result is formulated for quasi boundary triples here, and the assumption that the intersection of A and B is densely defined is dropped. The proof is similar to the one in [17], although more technical. For the convenience of the reader we give a self-contained complete proof in Sect. 4.

Theorem 3.1. *Let A and B be self-adjoint operators in $\mathfrak{H}$, suppose that the closed symmetric operator $S = A \cap B$ is simple, choose a quasi boundary triple $\{\mathcal{G}, \Gamma_0, \Gamma_1\}$ for $\overline{T} = S^*$ such that $A = \ker \Gamma_0$ and $B = \ker \Gamma_1$ as in Proposition 2.4, and let γ and M be the corresponding γ-field and Weyl function M, respectively. Assume that*

$$\overline{\gamma(\lambda_0)} \in \mathfrak{S}_2(\mathcal{G}, \mathfrak{H}) \quad \text{for some} \quad \lambda_0 \in \rho(A),$$

and that $\overline{M(\lambda_1)}$ is boundedly invertible in $\mathcal{G}$ for some $\lambda_1 \in \rho(A) \cap \rho(B)$. Then the following holds.

(i) *The resolvent difference of B and A is a trace class operator, that is,*

$$(B - \lambda)^{-1} - (A - \lambda)^{-1} \in \mathfrak{S}_1(\mathfrak{H}), \qquad \lambda \in \rho(A) \cap \rho(B).$$

(ii) *For all $\lambda \in \rho(A) \cap \rho(B)$ the closure of the Weyl function $\overline{M(\lambda)}$ exists and is boundedly invertible. Moreover, $L(\lambda) := \overline{M(\lambda) - \mathrm{Re}\, M(i)}$, $\lambda \in \rho(A)$, is a Nevanlinna function such that the limit $\overline{L(\lambda + i0)} = \lim_{y \downarrow 0} \overline{L(\lambda + iy)}$ exists in the operator norm for a.e. $\lambda \in \mathbb{R}$ and*

$$\overline{M(\lambda + i0)} := \overline{\mathrm{Re}\, M(i)} + L(\lambda + i0)$$

is boundedly invertible for a.e. $\lambda \in \mathbb{R}$.

(iii) *The space $L^2(\mathbb{R}, d\lambda, \mathcal{G}_\lambda)$, where $\mathcal{G}_\lambda := \overline{\mathrm{ran}\big(\overline{\mathrm{Im}\, M(\lambda + i0)}\big)}$ for a.e. $\lambda \in \mathbb{R}$, forms a spectral representation of A^{ac} such that the matrix $\{S_{AB}(\lambda)\}_{\lambda \in \mathbb{R}}$ of the scattering system $\{A, B\}$ admits the representation*

$$S_{AB}(\lambda) = I_{\mathcal{G}_\lambda} - 2i \sqrt{\overline{\mathrm{Im}\, M(\lambda + i0)}} \left(\overline{M(\lambda + i0)}\right)^{-1} \sqrt{\overline{\mathrm{Im}\, M(\lambda + i0)}}$$

for a.e. $\lambda \in \mathbb{R}$.

In Theorem 3.1 it is assumed that the closed symmetric operator $S = A \cap B$ is simple. This assumption can be dropped and Theorem 3.1 admits a natural generalization, which will be explained next. If S is not simple then there is a nontrivial orthogonal decomposition of $\mathfrak{H} = \mathfrak{H}_1 \oplus \mathfrak{H}_2$ such that

$$S = H_1 \oplus H_2,$$

where H_1 is a simple symmetric operator in $\mathfrak{H}_1$ and H_2 is a self-adjoint operator in $\mathfrak{H}_2$. Then there exist self-adjoint extensions A_1 and B_1 of H_1 in $\mathfrak{H}_1$ such that

$$A = A_1 \oplus H_2 \qquad \text{and} \qquad B = B_1 \oplus H_2.$$

Let $L^2(\mathbb{R}, d\lambda, \mathcal{H}_\lambda)$ be a spectral representation of the absolutely continuous part H_2^{ac} of the self-adjoint operator H_2 in $\mathfrak{H}_2$. Then the following variant of Theorem 3.1 holds.

Theorem 3.2. *Let A and B be self-adjoint operators in $\mathfrak{H}$, let $S = A \cap B$, choose a quasi boundary triple $\Pi = \{\mathcal{G}, \Gamma_0, \Gamma_1\}$ for $\overline{T} = S^*$ such that $A = \ker \Gamma_0$ and $B = \ker \Gamma_1$ as in Proposition* 2.4*, and let γ and M be the corresponding γ-field and Weyl function M, respectively. Assume that*

$$\overline{\gamma(\lambda_0)} \in \mathfrak{S}_2(\mathcal{G}, \mathfrak{H}) \quad \text{for some} \quad \lambda_0 \in \rho(A),$$

and that $\overline{M(\lambda_1)}$ is boundedly invertible in $\mathcal{G}$ for some $\lambda_1 \in \rho(A) \cap \rho(B)$. Then the conclusions (i) *and* (ii) *of Theorem* 3.1 *are valid and instead* (iii) *the following holds.*

(iii') *The space $L^2(\mathbb{R}, d\lambda, \mathcal{G}_\lambda \oplus \mathcal{H}_\lambda)$, where $\mathcal{G}_\lambda := \overline{\operatorname{ran}\bigl(\overline{\operatorname{Im} M(\lambda + i0)}\bigr)}$ for a.e. $\lambda \in \mathbb{R}$ forms a spectral representation of A^{ac} and the scattering matrix $\{S_{AB}(\lambda)\}_{\lambda \in \mathbb{R}}$ of the scattering system $\{A, B\}$ admits the representation*

$$S_{AB}(\lambda) = \begin{pmatrix} S_{A_1 B_1}(\lambda) & 0 \\ 0 & I_{\mathcal{H}_\lambda} \end{pmatrix}$$

for a.e. $\lambda \in \mathbb{R}$, where $\{S_{A_1 B_1}(\lambda)\}_{\lambda \in \mathbb{R}}$ given in Theorem 3.1 (iii) *is the scattering matrix of the scattering system $\{A_1, B_1\}$.*

4. Proof of Theorem 3.1

The proof of Theorem 3.1 is split into steps. First we make clear in Lemma 4.1 and Lemma 4.2 in which sense the limits $M(\lambda \pm i0)$ and $\operatorname{Im} M(\lambda \pm i0)$ of the Weyl function M and its imaginary part are understood; cf. Theorem 3.1 (ii) and (iii).

Lemma 4.1. *Let M be the Weyl function corresponding to the quasi boundary triple $\Pi = \{\mathcal{G}, \Gamma_0, \Gamma_1\}$ of Theorem* 3.1*. Then $\overline{\operatorname{Im} M(\lambda)} \in \mathfrak{S}_1(\mathcal{G})$ for all $\lambda \in \rho(A)$ and the limit*

$$\overline{\operatorname{Im} M(\lambda + i0)} := \lim_{\varepsilon \to +0} \overline{\operatorname{Im} M(\lambda + i\varepsilon)} \tag{4.1}$$

exists for a.e. $\lambda \in \mathbb{R}$ in $\mathfrak{S}_1(\mathcal{G})$.

Proof. From Proposition 2.2 (i) and the assumption $\overline{\gamma(\lambda_0)} \in \mathfrak{S}_2(\mathcal{G}, \mathfrak{H})$ for some $\lambda_0 \in \rho(A)$ it follows that $\overline{\gamma(\lambda)} \in \mathfrak{S}_2(\mathcal{G}, \mathfrak{H})$ for all $\lambda \in \rho(A)$. Hence we also have $\gamma(\lambda)^* \in \mathfrak{S}_2(\mathfrak{H}, \mathcal{G})$ and therefore Proposition 2.2 (v) yields

$$\overline{\operatorname{Im} M(\lambda)} = \operatorname{Im}(\lambda)\, \gamma(\lambda)^* \overline{\gamma(\lambda)} \in \mathfrak{S}_1(\mathcal{G}), \qquad \lambda \in \rho(A).$$

In particular, it follows that the limit in (4.1) exists for a.e. $\lambda \in \mathbb{R}$ in $\mathfrak{S}_1(\mathcal{G})$; cf. [18, 19, 38] or [28, Theorem 2.2]. □

Lemma 4.2. *Let M be the Weyl function corresponding to the quasi boundary triple $\Pi = \{\mathcal{G}, \Gamma_0, \Gamma_1\}$ in Theorem* 3.1*. For all $\varphi \in \operatorname{ran} \Gamma_0$ and a.e. $\lambda \in \mathbb{R}$ the limit*

$$M(\lambda \pm i0)\varphi := \lim_{\varepsilon \to +0} M(\lambda \pm i\varepsilon)\varphi \tag{4.2}$$

exists and the operator $M(\lambda \pm i0)$ *with* $\operatorname{dom} M(\lambda \pm i0) = \operatorname{ran}\Gamma_0$ *is closable. Moreover, for a.e.* $\lambda \in \mathbb{R}$ *the closure* $\overline{M(\lambda + i0)}$ *is boundedly invertible and*

$$\big(\overline{M(\lambda+i0)}\big)^{-1} = \lim_{\varepsilon\to 0+} \overline{M(\lambda+i\varepsilon)^{-1}} = \lim_{\varepsilon\to +0}\big(\overline{M(\lambda+i\varepsilon)}\big)^{-1} \tag{4.3}$$

holds in the operator norm for a.e. $\lambda \in \mathbb{R}$.

Proof. In order to see that the limit in (4.2) exists and defines a closable operator in $\mathcal{G}$ we recall that $M(\lambda)$, $\lambda \in \rho(A)$, admits the representation

$$M(\lambda)\varphi = \operatorname{Re} M(i)\varphi + L(\lambda)\varphi$$

for $\varphi \in \operatorname{ran}\Gamma_0$, see Proposition 2.2 (v). Since $\overline{\gamma(\lambda_0)} \in \mathfrak{S}_2(\mathcal{G},\mathfrak{H})$ by assumption we also have $\overline{\gamma(i)} \in \mathfrak{S}_2(\mathcal{G},\mathfrak{H})$ by Proposition 2.2 (i). Hence [9, Proposition 3.14] yields that the limits $L(\lambda \pm i0)$ of $L(\lambda \pm i\varepsilon)$ exist as $\varepsilon \to +0$ with respect to the Hilbert–Schmidt norm for a.e. $\lambda \in \mathbb{R}$. In particular, one has $L(\lambda \pm i0) \in \mathfrak{S}_2(\mathcal{G})$ for a.e. $\lambda \in \mathbb{R}$. Hence definition (4.2) makes sense and yields the representation

$$M(\lambda \pm i0)\varphi = \operatorname{Re} M(i)\varphi + L(\lambda \pm i0)\varphi$$

for all $\varphi \in \operatorname{dom} M(\lambda \pm i0) := \operatorname{ran}\Gamma_0$ and a.e. $\lambda \in \mathbb{R}$; thus there is a Borel set $\Lambda \subset \mathbb{R}$ of Lebesgue measure zero such that for each $\lambda \in \mathbb{R}\setminus\Lambda$ the limit operator $M(\lambda \pm i0)$ is well defined. The operators $M(\lambda \pm i0)$ are closable for a.e. $\lambda \in \mathbb{R}$ and the closures $\overline{M(\lambda \pm i0)}$ are given by

$$\overline{M(\lambda \pm i0)}\varphi = \overline{\operatorname{Re} M(i)}\varphi + L(\lambda \pm i0)\varphi \tag{4.4}$$

for all $\varphi \in \operatorname{dom}\overline{M(\lambda \pm i0)} = \operatorname{dom}\overline{\operatorname{Re} M(i)}$ and a.e. $\lambda \in \mathbb{R}$.

It will be shown next that the closures in (4.4) are boundedly invertible for a.e. $\lambda \in \mathbb{R}$ and that (4.3) holds in the operator norm for a.e. $\lambda \in \mathbb{R}$. Let us observe first that $\overline{M(\lambda)}$ is boundedly invertible for all $\lambda \in \rho(A)\setminus\mathcal{D}$, where $\mathcal{D}$ is a discrete subset of $\rho(A)$. In fact, since by our assumption there is some $\lambda_1 \in \rho(A)$ such that $\overline{M(\lambda_1)}$ is boundedly invertible it follows from Proposition 2.2 (v) that

$$\begin{aligned}\overline{M(\lambda)} &= \overline{M(\lambda_1)} + (\lambda - \overline{\lambda}_1)\gamma(\overline{\lambda}_1)^*\overline{\gamma(\lambda)}\\ &= \overline{M(\lambda_1)}\big[I - (\overline{\lambda}_1 - \lambda)\overline{M(\lambda_1)}^{-1}\gamma(\overline{\lambda}_1)^*\overline{\gamma(\lambda)}\big]\end{aligned}$$

holds for all $\lambda \in \rho(A)$. Furthermore, the operator-valued function

$$\lambda \mapsto (\overline{\lambda}_1 - \lambda)\overline{M(\lambda_1)}^{-1}\gamma(\overline{\lambda}_1)^*\overline{\gamma(\lambda)}$$

is holomorphic on $\rho(A)$ by Proposition 2.2 (i) and hence the analytic Fredholm theorem (see, e.g., [44, Theorem VI.14]) implies that

$$\overline{M(\lambda)}^{-1} = \big[I - (\overline{\lambda}_1 - \lambda)\overline{M(\lambda_1)}^{-1}\gamma(\overline{\lambda}_1)^*\overline{\gamma(\lambda)}\big]^{-1}\overline{M(\lambda_1)}^{-1}$$

is a bounded operator for all $\lambda \in \rho(A)\setminus\mathcal{D}$, where $\mathcal{D}$ is a discrete subset of $\rho(A)$.

Note that the transposed triple $\Pi^\top = \{\mathcal{G}, \Gamma_1, -\Gamma_0\}$ is also a quasi boundary triple. The corresponding γ-field $\gamma^\top$ and Weyl function $M^\top$ are given by

$$\lambda \mapsto \gamma^\top(\lambda) = \gamma(\lambda)M(\lambda)^{-1} \quad \text{and} \quad \lambda \mapsto M^\top(\lambda) = -M(\lambda)^{-1},$$

for $\lambda \in \rho(A) \cap \rho(B)$, respectively. Hence $\overline{M^\top(\lambda)}$ is boundedly invertible for any $\lambda \in \rho(A) \cap \rho(B)$ and

$$\overline{M(\lambda)}\,\overline{M^\top(\lambda)} = \overline{M^\top(\lambda)}\,\overline{M(\lambda)} = -I, \quad \lambda \in \rho(A) \cap \rho(B).$$

Since $M^\top$ is the Weyl function of $\Pi^\top = \{\mathcal{G}, \Gamma_1, -\Gamma_0\}$ Proposition 2.2 (v) yields the representation

$$M^\top(\lambda)\varphi = \operatorname{Re} M^\top(i)\varphi + \gamma^\top(i)^*\big(\lambda + (\lambda^2+1)(B-\lambda)^{-1}\big)\gamma^\top(i)\varphi$$

for $\varphi \in \operatorname{ran}\Gamma_1$, and hence

$$K(\lambda) := \overline{M^\top(\lambda)} = \overline{\operatorname{Re} M^\top(i)} + L^\top(\lambda), \qquad \lambda \in \rho(A) \cap \rho(B),$$

where

$$L^\top(\lambda) := \gamma^\top(i)^*\big(\lambda + (\lambda^2+1)(B-\lambda)^{-1}\big)\overline{\gamma^\top(i)}.$$

Our assumptions in Theorem 3.1 yield $\overline{\gamma^\top(i)} = \overline{\gamma(i)}\,\overline{M(i)}^{-1} \in \mathfrak{S}_2(\mathcal{G},\mathfrak{H})$ and $\gamma^\top(i)^* \in \mathfrak{S}_2(\mathfrak{H},\mathcal{G})$, and therefore we conclude from [9, Proposition 3.14] that the limits $K(\lambda + i0)$ of $K(\lambda + i\varepsilon)$ as $\varepsilon \to +0$ exist for a.e. $\lambda \in \mathbb{R}$ in the operator norm. Hence we get

$$K(\lambda+i0)\overline{M(\lambda+i0)} = \overline{M(\lambda+i0)}K(\lambda+i0) = -I$$

for a.e. $\lambda \in \mathbb{R}$ and it follows that the operator $\overline{M(\lambda+i0)}$ is boundedly invertible for a.e. $\lambda \in \mathbb{R}$. □

The remaining part of the proof of Theorem 3.1 is similar to the proof of [15, Theorem 3.8] and [17, Theorem 3.1]. The idea is mainly based on Theorem 4.3 below, which follows from [9, Theorem 18.4]; cf. [17, Theorem A.2]. Some of the arguments require special care when working in the more general context of quasi boundary triples since the values of the γ-field and Weyl function are not closed operators in general; we provide the full details whenever necessary. In the following we shall denote by $\mathcal{L}(\mathcal{G})$ the space of bounded and everywhere defined operators in $\mathcal{G}$.

Theorem 4.3. *Assume that the self-adjoint operators A and B satisfy the trace class condition* (3.1) *and suppose that the resolvent difference admits the factorization*

$$(B-i)^{-1} - (A-i)^{-1} = \phi(A)CGC^* = QC^*,$$

where $C \in \mathfrak{S}_2(\mathcal{G},\mathfrak{H})$, let $\phi : \mathbb{R} \to \mathbb{R}$ be a bounded continuous function and let $Q = \phi(A)CG$. Assume that

$$\mathfrak{H}^{ac}(A) = \operatorname{clsp}\big\{E_A^{ac}(\delta)[\operatorname{ran} C] : \delta \in \mathcal{B}(\mathbb{R})\big\} \tag{4.5}$$

holds and let $D(\lambda) = \frac{d}{d\lambda}C^*E_A((-\infty,\lambda))C$ and $\mathcal{G}_\lambda = \overline{\operatorname{ran} D(\lambda)}$ for a.e. $\lambda \in \mathbb{R}$. Then $L^2(\mathbb{R}, d\lambda, \mathcal{G}_\lambda)$ is a spectral representation of A^{ac} and the scattering matrix of the scattering system $\{A, B\}$ is given by

$$S_{AB}(\lambda) = I_{\mathcal{G}_\lambda} + 2\pi i(1+\lambda^2)^2\sqrt{D(\lambda)}Z(\lambda)\sqrt{D(\lambda)}$$

for a.e. $\lambda \in \mathbb{R}$, *where*

$$Z(\lambda) = \frac{1}{\lambda + i} Q^* Q + \frac{1}{(\lambda + i)^2} \phi(\lambda) G + \lim_{\varepsilon \to +0} Q^* \big(B - (\lambda + i\varepsilon)\big)^{-1} Q$$

and the limit of the last term on the right hand side exists in the Hilbert–Schmidt norm.

Proof of Theorem 3.1. (i) Since $\overline{\gamma(\lambda_0)} \in \mathfrak{S}_2(\mathcal{G}, \mathfrak{H})$ for some $\lambda_0 \in \rho(A)$ and $M(\lambda_1)^{-1}$ is bounded for some $\lambda_1 \in \rho(A) \cap \rho(B)$ it follows from [13, Proposition 3.5] that $\overline{\gamma(\lambda)} \in \mathfrak{S}_2(\mathcal{G}, \mathfrak{H})$ for all $\lambda \in \rho(A)$ and $M(\lambda)^{-1}$ is bounded for all $\lambda \in \rho(A) \cap \rho(B)$; cf. the proofs of Lemmas 4.1 and 4.2. Then we also have $\gamma(\overline{\lambda})^* \in \mathfrak{S}_2(\mathfrak{H}, \mathcal{G})$ for all $\lambda \in \rho(A)$ and hence the resolvent difference

$$(B - \lambda)^{-1} - (A - \lambda)^{-1} = -\gamma(\lambda) M(\lambda)^{-1} \gamma(\overline{\lambda})^* = -\overline{\gamma(\lambda)}\, \overline{M(\lambda)^{-1}} \gamma(\overline{\lambda})^*$$

is a trace class operator for all $\lambda \in \rho(A) \cap \rho(B)$.

(ii) This statement follows from Lemma 4.2.

(iii) This item is proved in two separate steps. In the first step we find a preliminary form of the scattering matrix making use of Theorem 4.3. In the second step we then obtain the final form of the scattering matrix.

Step 1. Expressing the resolvent difference at $\lambda = i$ in the same way as in the proof of (i) and using $\gamma(i) = (A + i)(A - i)^{-1} \gamma(-i)$ we obtain

$$\begin{aligned} (B - i)^{-1} - (A - i)^{-1} &= -\overline{\gamma(i)}\, \overline{M(i)^{-1}} \gamma(-i)^* \\ &= -(A + i)(A - i)^{-1} \overline{\gamma(-i)}\, \overline{M(i)^{-1}} \gamma(-i)^* \\ &= \phi(A) C G C^*, \end{aligned}$$

where we have chosen

$$\phi(t) = \frac{t + i}{t - i}, \quad t \in \mathbb{R}, \qquad C = \overline{\gamma(-i)} \quad \text{and} \quad G = -\overline{M(i)^{-1}}.$$

It follows in exactly the same way as in [17, Proof of Theorem 3.1] that the condition (4.5) in Theorem 4.3 holds. Now we compute the $\mathcal{L}(\mathcal{G})$-valued function

$$\lambda \mapsto D(\lambda) = \frac{d}{d\lambda} C^* E_A((-\infty, \lambda)) C$$

and its square root $\lambda \mapsto \sqrt{D(\lambda)}$ for a.e. $\lambda \in \mathbb{R}$. First of all, we have

$$\begin{aligned} D(\lambda) &= \lim_{\varepsilon \to 0+} \frac{1}{2\pi i} C^* \big((A - \lambda - i\varepsilon)^{-1} - (A - \lambda + i\varepsilon)^{-1}\big) C \\ &= \lim_{\varepsilon \to 0+} \frac{\varepsilon}{\pi} C^* \big((A - \lambda - i\varepsilon)^{-1} (A - \lambda + i\varepsilon)^{-1}\big) C. \end{aligned}$$

On the other hand,

$$\operatorname{Im} M(\lambda + i\varepsilon) = \varepsilon \gamma(\lambda + i\varepsilon)^* \gamma(\lambda + i\varepsilon)$$

together with $\gamma(\lambda + i\varepsilon) = (A + i)(A - \lambda - i\varepsilon)^{-1} \gamma(-i)$ shows

$$\operatorname{Im} M(\lambda + i\varepsilon) = \varepsilon \gamma(-i)^* (I_{\mathfrak{H}} + A^2) \big(A - \lambda + i\varepsilon\big)^{-1} \big(A - \lambda - i\varepsilon\big)^{-1} \gamma(-i)$$

and hence we conclude

$$\overline{\operatorname{Im} M(\lambda+i\varepsilon)} = \varepsilon C^*(I_{\mathfrak{H}} + A^2)\bigl(A-\lambda+i\varepsilon\bigr)^{-1}\bigl(A-\lambda-i\varepsilon\bigr)^{-1}C.$$

This implies $\overline{\operatorname{Im} M(\lambda+i0)} = \lim_{\varepsilon\to 0+} \overline{\operatorname{Im} M(\lambda+i\varepsilon)} = \pi(1+\lambda^2)D(\lambda)$ for a.e. $\lambda\in\mathbb{R}$ and, in particular, $\operatorname{ran}(\overline{\operatorname{Im} M(\lambda+i0)}) = \operatorname{ran} D(\lambda)$ for a.e. $\lambda\in\mathbb{R}$, and hence

$$\mathcal{G}_\lambda = \overline{\operatorname{ran}\bigl(\overline{\operatorname{Im} M(\lambda+i0)}\bigr)} = \overline{\operatorname{ran} D(\lambda)} \quad \text{for a.e. } \lambda\in\mathbb{R}.$$

Therefore, Theorem 4.3 yields that $L^2(\mathbb{R}, d\lambda, \mathcal{G}_\lambda)$ is a spectral representation of A^{ac} and the scattering matrix $\{S_{AB}(\lambda)\}_{\lambda\in\mathbb{R}}$ is given by

$$\begin{aligned} S_{AB}(\lambda) &= I_{\mathcal{G}_\lambda} + 2\pi i(1+\lambda^2)^2\sqrt{D(\lambda)}Z(\lambda)\sqrt{D(\lambda)} \\ &= I_{\mathcal{G}_\lambda} + 2i(1+\lambda^2)\sqrt{\overline{\operatorname{Im} M(\lambda+i0)}}Z(\lambda)\sqrt{\overline{\operatorname{Im} M(\lambda+i0)}} \end{aligned} \tag{4.6}$$

for a.e. $\lambda\in\mathbb{R}$, where

$$Z(\lambda) = \frac{1}{\lambda+i}Q^*Q + \frac{1}{(\lambda+i)^2}\phi(\lambda)G + \lim_{\varepsilon\to 0+} Q^*\bigl(B-(\lambda+i\varepsilon)\bigr)^{-1}Q \tag{4.7}$$

and $Q = \phi(A)CG$ is given by

$$Q = -(A+i)(A-i)^{-1}\overline{\gamma(-i)}\,\overline{M(i)^{-1}} = -\overline{\gamma(i)}\,\overline{M(i)^{-1}} \in \mathfrak{S}_2(\mathcal{G},\mathfrak{H}).$$

Step 2. In this step we compute the explicit form

$$Z(\lambda) = -\frac{1}{1+\lambda^2}\overline{M(\lambda+i0)^{-1}} \tag{4.8}$$

for a.e. $\lambda\in\mathbb{R}$ of $Z(\lambda)$ in (4.7). From this and (4.6) the asserted form of the scattering matrix follows immediately.

Observe that by Proposition 2.4 we have

$$\begin{aligned} \Gamma_0(B-\lambda)^{-1} &= \Gamma_0(A-\lambda)^{-1} - \Gamma_0\gamma(\lambda)M(\lambda)^{-1}\gamma(\overline{\lambda})^* \\ &= -M(\lambda)^{-1}\gamma(\overline{\lambda})^* \\ &= -\overline{M(\lambda)^{-1}}\gamma(\overline{\lambda})^* \end{aligned}$$

for $\lambda\in\rho(A)\cap\rho(B)$ and hence

$$\begin{aligned} \Gamma_0(B+i)^{-1} &= -\overline{M(-i)^{-1}}\gamma(i)^* \\ &= \bigl(-\overline{\gamma(i)}(M(-i)^{-1})^*\bigr)^* \\ &= \bigl(-\overline{\gamma(i)}\,\overline{M(i)^{-1}}\bigr)^* \\ &= Q^*, \end{aligned}$$

where we have used $(M(-i)^{-1})^* = (M(-i)^*)^{-1} = \overline{M(i)^{-1}}$. This yields

$$\begin{aligned} Q^*(B-\lambda)^{-1}Q &= \Gamma_0(B+i)^{-1}(B-\lambda)^{-1}Q \\ &= \Gamma_0\bigl(Q^*(B-\overline{\lambda})^{-1}(B-i)^{-1}\bigr)^* \\ &= \Gamma_0\bigl(\Gamma_0(B+i)^{-1}(B-\overline{\lambda})^{-1}(B-i)^{-1}\bigr)^*. \end{aligned} \tag{4.9}$$

Since

$$(B+i)^{-1}(B-\overline{\lambda})^{-1}(B-i)^{-1} = \frac{-1}{1+\overline{\lambda}^2}\big((B+i)^{-1}-(B-\overline{\lambda})^{-1}\big) + \frac{1}{2i(\overline{\lambda}-i)}\big((B+i)^{-1}-(B-i)^{-1}\big)$$

it follows from Proposition 2.4 that

$$\Gamma_0(B+i)^{-1}(B-\overline{\lambda})^{-1}(B-i)^{-1} = \frac{1}{1+\overline{\lambda}^2}\big(M(-i)^{-1}\gamma(i)^* - M(\overline{\lambda})^{-1}\gamma(\lambda)^*\big) - \frac{1}{2i(\overline{\lambda}-i)}\big(M(-i)^{-1}\gamma(i)^* - M(i)^{-1}\gamma(-i)^*\big).$$

Taking into account $(M(\overline{\mu})^{-1})^* = \overline{M(\mu)^{-1}}$ for $\mu \in \rho(A)\cap\rho(B)$ we obtain for the adjoint

$$\big(\Gamma_0(B+i)^{-1}(B-\overline{\lambda})^{-1}(B-i)^{-1}\big)^* = \frac{1}{1+\lambda^2}\big(\overline{\gamma(i)}\,\overline{M(i)^{-1}} - \overline{\gamma(\lambda)}\,\overline{M(\lambda)^{-1}}\big) + \frac{1}{2i(\lambda+i)}\big(\overline{\gamma(i)}\,\overline{M(i)^{-1}} - \overline{\gamma(-i)}\,\overline{M(-i)^{-1}}\big)$$

and for $\varphi \in \operatorname{ran}\Gamma_1 = \operatorname{dom} M(\mu)^{-1}$, $\mu \in \rho(A)\cap\rho(B)$, we then conclude from (4.9)

$$\begin{aligned} Q^*(B-\lambda)^{-1}Q\varphi &= \Gamma_0\big(\Gamma_0(B+i)^{-1}(B-\overline{\lambda})^{-1}(B-i)^{-1}\big)^*\varphi \\ &= \frac{1}{1+\lambda^2}\Gamma_0\big(\gamma(i)M(i)^{-1} - \gamma(\lambda)M(\lambda)^{-1}\big)\varphi \\ &\quad + \frac{1}{2i(\lambda+i)}\Gamma_0\big(\gamma(i)M(i)^{-1} - \gamma(-i)M(-i)^{-1}\big)\varphi \\ &= \frac{1}{1+\lambda^2}\big(M(i)^{-1} - M(\lambda)^{-1}\big)\varphi \\ &\quad + \frac{1}{2i(\lambda+i)}\big(M(i)^{-1} - M(-i)^{-1}\big)\varphi, \end{aligned}$$

which extends by continuity from the dense set $\operatorname{ran}\Gamma_1$ onto $\mathcal{G}$ and takes the form

$$Q^*(B-\lambda)^{-1}Q = \frac{1}{1+\lambda^2}\big(\overline{M(i)^{-1}} - \overline{M(\lambda)^{-1}}\big) + \frac{1}{2i(\lambda+i)}\big(\overline{M(i)^{-1}} - \overline{M(-i)^{-1}}\big).$$

This leads to

$$\lim_{\varepsilon\to 0+} Q^*\big(B-(\lambda+i\varepsilon)\big)^{-1}Q = \frac{1}{1+\lambda^2}\big(\overline{M(i)^{-1}} - \overline{M(\lambda+i0)^{-1}}\big) + \frac{1}{2i(\lambda+i)}\big(\overline{M(i)^{-1}} - \overline{M(-i)^{-1}}\big)$$

for a.e. $\lambda \in \mathbb{R}$. Note also that by Lemma 4.2 the limit $\overline{M(\lambda+i0)^{-1}}$ exists for a.e. $\lambda \in \mathbb{R}$ in the operator norm.

Moreover, for $\varphi \in \operatorname{ran} \Gamma_1 = \operatorname{dom} M(\mu)^{-1}$, $\mu \in \rho(A) \cap \rho(B)$, we have

$$\begin{aligned}
Q^* Q\varphi &= \left(\overline{\gamma(i)}\, \overline{M(i)^{-1}}\right)^* \overline{\gamma(i)}\, \overline{M(i)^{-1}}\varphi \\
&= \overline{M(-i)^{-1}} \gamma(i)^* \gamma(i) M(i)^{-1} \varphi \\
&= \frac{1}{2i} M(-i)^{-1} \big(M(i) - M(-i)\big) M(i)^{-1} \varphi \\
&= \frac{1}{2i} \big(M(-i)^{-1} - M(i)^{-1}\big)\varphi.
\end{aligned}$$

Hence we obtain for $\varphi \in \operatorname{ran} \Gamma_1$ and a.e. $\lambda \in \mathbb{R}$ that

$$\begin{aligned}
Z(\lambda)\varphi = &\frac{1}{\lambda + i} Q^* Q \varphi + \frac{1}{(\lambda + i)^2} \phi(\lambda) G \varphi + Q^* \big(B - (\lambda + i0)\big)^{-1} Q \varphi \\
= &\frac{1}{2i(\lambda + i)} \big(M(-i)^{-1} - M(i)^{-1}\big)\varphi - \frac{1}{1 + \lambda^2} M(i)^{-1} \varphi \\
&+ \frac{1}{1 + \lambda^2} \big(M(i)^{-1} - \overline{M(\lambda + i0)^{-1}}\big)\varphi + \frac{1}{2i(\lambda + i)} \big(M(i)^{-1} - M(-i)^{-1}\big)\varphi \\
= &- \frac{1}{1 + \lambda^2} \overline{M(\lambda + i0)^{-1}} \varphi
\end{aligned}$$

and since $\overline{M(\lambda + i0)^{-1}} \in \mathcal{L}(\mathcal{G})$ we conclude (4.8). This completes the proof of Theorem 3.1. □

5. An example

In this section we discuss a scattering system consisting of the one-dimensional Schrödinger operators $\{A, B\}$, where

$$Af = -f'', \quad Bf = -f'' + Vf, \quad \operatorname{dom} A = \operatorname{dom} B = H^2(\mathbb{R}). \tag{5.1}$$

Our aim is to show in a particularly simple situation how quasi boundary triples for the adjoints of non-densely defined symmetric operators appear and can be applied to obtain a formula for the scattering matrix via Theorem 3.1. To avoid technical difficulties we will assume that the real-valued potential V in (5.1) satisfies the condition

$$V \in L^\infty(\mathbb{R}). \tag{5.2}$$

It is well known that the operators A and B in (5.1) are self-adjoint in $L^2(\mathbb{R})$. Later, in Lemma 5.2, it will also be assumed that $V \in L^1(\mathbb{R})$. In the present situation the symmetric operator $S = A \cap B$ has the form

$$Sf = -f'' = -f'' + Vf, \quad \operatorname{dom} S = \big\{ f \in H^2(\mathbb{R}) : Vf = 0 \big\}, \tag{5.3}$$

and, in general, S is not densely defined. In particular, it may happen that $\operatorname{dom} S = \{0\}$. In the following we use the factorization

$$V = \sqrt{|V|}\, \operatorname{sgn}(V) \sqrt{|V|} = D^* U D, \tag{5.4}$$

where $D : L^2(\mathbb{R}) \to \mathcal{G}$, $f \mapsto \sqrt{|V|}f$, $\mathcal{G} := \overline{\operatorname{ran}\sqrt{|V|}}$, and $U : \mathcal{G} \to \mathcal{G}$, $\varphi \mapsto \operatorname{sgn}(V)\varphi$. Observe that $\operatorname{ran} D$ is dense in $\mathcal{G}$ and that U is a unitary operator in $\mathcal{G}$. In the next proposition we shall construct a suitable quasi boundary triple for the adjoint relation S^*. For our purposes it is convenient to introduce the linear relation

$$T = \bigl\{\{f, -f'' + Vh\} : f, h \in H^2(\mathbb{R})\bigr\}$$

in $L^2(\mathbb{R}) \times L^2(\mathbb{R})$. It is not difficult to see that $T = A \widehat{+} B$ holds. We emphasize that the quasi boundary triple $\Pi = \{\mathcal{G}, \Gamma_0, \Gamma_1\}$ below is not a generalized boundary triple in the sense of [23, Definition 6.1] whenever $\operatorname{ran} D$ is not closed.

Proposition 5.1. *Let A, B and S, T be as above. Then $\Pi = \{\mathcal{G}, \Gamma_0, \Gamma_1\}$, where*

$$\mathcal{G} = \overline{\operatorname{ran}\sqrt{|V|}}, \quad \Gamma_0 \widehat{f} = Dh \quad \textit{and} \quad \Gamma_1 \widehat{f} = UDh - UDf,$$

$\widehat{f} = \{f, -f'' + Vh\} \in T$, is a quasi boundary triple for $\overline{T} = S^*$ such that $A = \ker \Gamma_0$ and $B = \ker \Gamma_1$. The corresponding γ-field and Weyl function are given by

$$\gamma(\lambda)\varphi = -(A - \lambda)^{-1} D^* \varphi, \quad \varphi \in \operatorname{ran} \Gamma_0,$$

and

$$M(\lambda)\varphi = U\varphi + UD(A - \lambda)^{-1} D^* U \varphi, \quad \varphi \in \operatorname{ran} \Gamma_0.$$

Proof. Consider two elements $\widehat{f} = \{f, -f'' + Vh\}$, $\widehat{g} = \{g, -g'' + Vk\} \in T$ and note that $(-f'', g)_{L^2(\mathbb{R})} - (f, -g'')_{L^2(\mathbb{R})} = 0$ as $f, g \in H^2(\mathbb{R}) = \operatorname{dom} A$ and A is a self-adjoint operator. A straightforward computation shows

$$\begin{aligned}
&\bigl(-f'' + Vh, g\bigr)_{L^2(\mathbb{R})} - \bigl(f, -g'' + Vk\bigr)_{L^2(\mathbb{R})} \\
&\quad = (Vh, g)_{L^2(\mathbb{R})} - (f, Vk)_{L^2(\mathbb{R})} \\
&\quad = (h, Vg)_{L^2(\mathbb{R})} - (Vf, k)_{L^2(\iota)} + (Vh, k)_{L^2(\mathbb{R})} - (h, Vk)_{L^2(\mathbb{R})} \\
&\quad = \bigl(Vh - Vf, k\bigr)_{L^2(\mathbb{R})} - \bigl(h, Vk - Vg\bigr)_{L^2(\mathbb{R})} \\
&\quad = \bigl(UDh - UDf, Dk\bigr)_{\mathcal{G}} - \bigl(Dh, UDk - UDg\bigr)_{\mathcal{G}} \\
&\quad = (\Gamma_1 \widehat{f}, \Gamma_0 \widehat{g})_{\mathcal{G}} - (\Gamma_0 \widehat{f}, \Gamma_1 \widehat{g})_{\mathcal{G}}
\end{aligned}$$

and hence the abstract Green's identity in Definition 2.1 is satisfied. Next we check that $\operatorname{ran}(\Gamma_0, \Gamma_1)^\top$ is dense in $\mathcal{G} \times \mathcal{G}$. Assume that for some $\zeta, \xi \in \mathcal{G}$ we have

$$0 = (\zeta, \Gamma_0 \widehat{f})_{\mathcal{G}} + (\xi, \Gamma_1 \widehat{f})_{\mathcal{G}} = (\zeta, Dh)_{\mathcal{G}} + (\xi, UDh - UDf)_{\mathcal{G}} \tag{5.5}$$

for all $\widehat{f} = \{f, -f'' + Vh\} \in T$. In particular, if $h = 0$ then

$$0 = (\xi, UDf)_{\mathcal{G}} = (D^* U^* \xi, f)_{L^2(\mathbb{R})}$$

for all $f \in H^2(\mathbb{R})$. Hence $D^* U^* \xi = 0$ and $\ker D^* = (\operatorname{ran} D)^\perp = \{0\}$ yields $U^* \xi = 0$. But U is unitary and thus we conclude $\xi = 0$. Now (5.5) reduces to $0 = (\zeta, Dh)_{\mathcal{G}} = (D^* \zeta, h)_{L^2(\mathbb{R})}$ for all $h \in H^2(\mathbb{R})$. As above $\ker D^* = \{0\}$ implies $\zeta = 0$. We have shown that $\operatorname{ran}(\Gamma_0, \Gamma_1)^\top$ is dense in $\mathcal{G} \times \mathcal{G}$.

Furthermore, if $\widehat{f} \in \ker \Gamma_0$ then $Dh = 0$ for all $h \in H^2(\mathbb{R})$, and hence $Vh = 0$ for all $h \in H^2(\mathbb{R})$ by (5.4). Therefore

$$\ker \Gamma_0 = \big\{\{f, -f''\} : f \in H^2(\mathbb{R})\big\} = A$$

and it follows that $\Pi = \{\mathcal{G}, \Gamma_0, \Gamma_1\}$ is a quasi boundary triple for $\overline{T} = S^*$. Moreover, if $\widehat{f} \in \ker \Gamma_1$ then $Dh = Df$ and hence $Vh = Vf$ by (5.4). This implies

$$\ker \Gamma_1 = \big\{\{f, -f'' + Vf\} : f \in H^2(\mathbb{R})\big\} = B.$$

It remains to verify the assertions on the form of the γ-field and Weyl function corresponding to the quasi boundary triple $\Pi = \{\mathcal{G}, \Gamma_0, \Gamma_1\}$. Note first that in the present situation for $\lambda \in \rho(A)$ we have

$$\widehat{\mathcal{N}}_\lambda(T) = \big\{\{f_\lambda, \lambda f_\lambda\} : f_\lambda = -(A-\lambda)^{-1}Vh,\ h \in H^2(\mathbb{R})\big\}.$$

As

$$\lambda f_\lambda = -\lambda(A-\lambda)^{-1}Vh = -A(A-\lambda)^{-1}Vh + Vh = Af_\lambda + Vh,$$

it follows that the elements $\widehat{f}_\lambda \in \widehat{\mathcal{N}}_\lambda(T)$ have the form

$$\widehat{f}_\lambda = \big\{f_\lambda, -f_\lambda'' + Vh\big\}, \quad f_\lambda = -(A-\lambda)^{-1}Vh.$$

Using (5.4) we find

$$\widehat{f}_\lambda = \big\{f_\lambda, -f_\lambda'' + D^*UDh\big\}, \quad f_\lambda = -(A-\lambda)^{-1}D^*UDh. \tag{5.6}$$

Setting $\varphi = Dh \in \operatorname{ran}\Gamma_0$, $h \in H^2(\mathbb{R})$, we get

$$\widehat{f}_\lambda = \big\{f_\lambda, -f_\lambda'' + D^*U\varphi\big\}, \quad f_\lambda = -(A-\lambda)^{-1}D^*U\varphi.$$

By definition one has $\Gamma_0\widehat{f}_\lambda = Dh = \varphi$ which yields

$$\gamma(\lambda)\varphi = f_\lambda = -(A-\lambda)^{-1}D^*U\varphi.$$

Hence the assertion on the γ-field is proven. Furthermore, applying Γ_1 to the same element in (5.6) gives $\Gamma_1\widehat{f}_\lambda = UDh - UDf_\lambda = U\varphi + UD(A-\lambda)^{-1}D^*U\varphi$, which implies the assertion on the Weyl function. □

In the next lemma we shall strengthen the condition (5.2) on V such that the assumptions on γ and M in Theorem 3.1 are satisfied.

Lemma 5.2. *Assume that the real-valued potential V in* (5.1) *satisfies*

$$V \in L^\infty(\mathbb{R}) \cap L^1(\mathbb{R}) \tag{5.7}$$

and let γ and M be the γ-field and Weyl function corresponding to the quasi boundary triple $\Pi = \{\mathcal{G}, \Gamma_0, \Gamma_1\}$ in Proposition 5.1. *Then*

$$\overline{\gamma(\lambda_0)} \in \mathfrak{S}_2\big(\mathcal{G}, L^2(\mathbb{R})\big) \tag{5.8}$$

for some $\lambda_0 \in \rho(A)$ and $\overline{M(\lambda_1)}$ is boundedly invertible for some $\lambda_1 \in \rho(A) \cap \rho(B)$.

Proof. The assumption (5.7) yields that $D(A-\overline{\lambda})^{-1}$ is a Hilbert–Schmidt operator for all $\lambda \in \rho(A)$. Hence $(A-\lambda)^{-1}D^*U$ is also a Hilbert–Schmidt operator and (5.8) follows for all $\lambda_0 \in \rho(A)$. Moreover, one has

$$\overline{M(\lambda)} = U + UD(A-\lambda)^{-1}D^*U, \quad \lambda \in \rho(A).$$

For $\mathrm{Im}(\lambda)$ sufficiently large the operator norm $UD(A-\lambda)^{-1}D^*U^*$ becomes small and hence $\overline{M(\lambda_1)}$ is boundedly invertible for some $\lambda_1 \in \rho(A) \cap \rho(B)$. □

Finally, we summarize the conclusion for the scattering matrix of the scattering system $\{A, B\}$. Here it is clear that the resolvent difference of A and B is a trace class operator (see, e.g., [47, Lemma 9.34]) and this also follows from Theorem 3.1. Furthermore, the symmetric operator S in (5.3) is simple and the absolutely continuous part A^{ac} of A coincides with A. Hence by Theorem 3.1 the scattering matrix $\{S_{AB}(\lambda)\}_{\lambda\in\mathbb{R}}$ of the scattering system $\{A, B\}$ admits the representation

$$S_{AB}(\lambda) = I_{\mathcal{G}_\lambda} - 2i\sqrt{\mathrm{Im}\, M(\lambda+i0)}\left(\overline{M(\lambda+i0)}\right)^{-1}\sqrt{\mathrm{Im}\, M(\lambda+i0)} \tag{5.9}$$

for a.e. $\lambda \in \mathbb{R}$, and $L^2(\mathbb{R}, d\lambda, \mathcal{G}_\lambda)$, where

$$\mathcal{G}_\lambda := \overline{\mathrm{ran}\big(\mathrm{Im}\, M(\lambda+i0)\big)} \tag{5.10}$$

for a.e. $\lambda \in \mathbb{R}$, is a spectral representation of A. It will turn out next that the limit $\mathrm{Im}\, M(\lambda+i0)$ is zero for a.e. $\lambda < 0$ and a rank two operator for a.e. $\lambda > 0$ and hence (5.10) simplifies to $\mathcal{G}_\lambda = \mathrm{ran}\big(\mathrm{Im}\, M(\lambda+i0)\big)$ and for the scattering matrix we get

$$S_{AB}(\lambda) = I_{\mathcal{G}_\lambda} - 2i\sqrt{\mathrm{Im}\, M(\lambda+i0)}\left(\overline{M(\lambda+i0)}\right)^{-1}\sqrt{\mathrm{Im}\, M(\lambda+i0)}.$$

In fact, for $\varphi \in H^2(\mathbb{R})$ we first compute $\mathrm{Im}\, M(\lambda+i0)\varphi$ for $\lambda \in \mathbb{R}$. Observe that for $\lambda \in \mathbb{C}\setminus\mathbb{R}$ we have

$$((A-\lambda)^{-1}f)(x) = \int_{\mathbb{R}} \frac{i}{2\sqrt{\lambda}} e^{i\sqrt{\lambda}|x-y|} f(y)dy, \quad f \in L^2(\mathbb{R}),$$

where the square root $\sqrt{\cdot}$ is defined for all $\lambda \in \mathbb{C}\setminus[0,\infty)$ such that $\mathrm{Im}\sqrt{\lambda} > 0$ and $\sqrt{\lambda} \geq 0$ for $\lambda \in [0,\infty)$. Making use of $\sqrt{\overline{\lambda}} = -\overline{\sqrt{\lambda}}$ for $\lambda \in \mathbb{C}\setminus[0,\infty)$ we find

$$\begin{aligned}(\mathrm{Im}\, M(\lambda)\varphi)(x) &= \frac{1}{2}\,\mathrm{sgn}(V(x))\sqrt{|V(x)|}\\ &\quad\times \int_{\mathbb{R}} \left[\frac{1}{2\sqrt{\lambda}} e^{i\sqrt{\lambda}|x-y|} + \frac{1}{2\overline{\sqrt{\lambda}}} e^{-i\overline{\sqrt{\lambda}}|x-y|}\right]\sqrt{|V(y)|}\,\mathrm{sgn}(V(y))\varphi(y)dy\end{aligned}$$

for $\lambda \in \mathbb{C} \setminus \mathbb{R}$ and for $\lambda + i0 = \lambda > 0$ this implies

$$\begin{aligned}
&(\operatorname{Im} M(\lambda + i0)\varphi)(x) \\
&= \frac{1}{2\sqrt{\lambda}} \operatorname{sgn}(V(x))\sqrt{|V(x)|} \int_{\mathbb{R}} \cos\bigl(\sqrt{\lambda}|x-y|\bigr)\sqrt{|V(y)|}\operatorname{sgn}(V(y))\varphi(y)dy \\
&= \frac{1}{2\sqrt{\lambda}} \operatorname{sgn}(V(x))\sqrt{|V(x)|}\cos(\sqrt{\lambda}x) \int_{\mathbb{R}} \cos(\sqrt{\lambda}y)\sqrt{|V(y)|}\operatorname{sgn}(V(y))\varphi(y)dy \\
&\quad + \frac{1}{2\sqrt{\lambda}} \operatorname{sgn}(V(x))\sqrt{|V(x)|}\sin(\sqrt{\lambda}x) \int_{\mathbb{R}} \sin(\sqrt{\lambda}y)\sqrt{|V(y)|}\operatorname{sgn}(V(y))\varphi(y)dy;
\end{aligned}$$

in particular, $\operatorname{Im} M(\lambda + i0)$ is a rank two operator for $\lambda > 0$ and the spaces $\mathcal{G}_\lambda$, $\lambda > 0$, in the spectral representation $L^2(\mathbb{R}, d\lambda, \mathcal{G}_\lambda)$ of A^{ac} are given by

$$\mathcal{G}_\lambda = \operatorname{span}\bigl\{\operatorname{sgn}(V)\sqrt{|V|}\cos(\sqrt{\lambda}\cdot), \operatorname{sgn}(V)\sqrt{|V|}\sin(\sqrt{\lambda}\cdot)\bigr\}.$$

Note that $\operatorname{Im} M(\lambda+i0) = 0$ for a.e. $\lambda < 0$ as $(-\infty, 0) \subset \rho(A)$, and hence $\mathcal{G}_\lambda = \{0\}$ for a.e. $\lambda < 0$.

Remark 5.3. (i) The representation (5.9) of the scattering matrix coincides with the one obtained in a different way in [9, Sect. 18.2.2].

(ii) Proposition 5.1 admits a straight forward generalization to higher dimensions. However, under the assumption (5.7) the condition (5.8) in Lemma 5.2 remains valid only for space dimensions $n = 2, 3$.

(iii) If $\operatorname{ran} D$ is not closed then the quasi boundary triple in Proposition 5.1 is not a generalized boundary triple and hence our extension of [17, Theorem 3.1] for quasi boundary triples is necessary here.

(iv) If for some $C > 0$ the condition

$$|V(x)| \leqslant C\frac{1}{(1+|x|)^{1+\varepsilon}}, \quad \varepsilon > 0,$$

is satisfied for a.e. $x \in \mathbb{R}^n$ it was shown by Kato in [30] (see also [31]) that the wave operators $W_\pm(B, A)$ exist and are complete. In this proof it also turns out that the limit $\overline{M(\lambda + i0)}$ of the function $\overline{M}$ exists for a.e. $\lambda \in \mathbb{R}$ in the operator norm.

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On the spectrum of the quantum Rabi model

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Dedicated to the memory of Boris Pavlov

Abstract. We investigate the behavior of large eigenvalues for the quantum Rabi Hamiltonian, i.e., for the Jaynes–Cummings model without the rotating wave approximation. The three-term asymptotics we obtain involves all the parameters of the model so that we can recover them from the behavior of its large eigenvalues.

1. Introduction

1.1. Preliminaries

The simplest interaction between a two-level atom and a classical light field is described by the Rabi model [15, 16]. In [12] the fully quantized version with the rotating-wave approximation (RWA) was considered by E.T. Jaynes and F.W. Cummings. In this paper we consider the quantum Rabi model [7] which is also called the Jaynes–Cummings model without the rotating-wave approximation. The model couples a quantized single-mode radiation and a two-level quantum system according to the idea that each photon creation accompanies atomic de-excitation, and each photon annihilation accompanies atomic excitation (see [18]). It is the simplest physical example of the interaction between radiation and matter which is a central problem in quantum optics. We refer to [18] for the microscopic derivation of the quantum Rabi model in Cavity Quantum Electrodynamics and to [14] for a list of recent works on the quantum Rabi model.

In the following, ω denotes the frequency of the quantized one-mode electromagnetic field. Then the corresponding Hamiltonian is a quantum quadratic oscillator and its eigenvalues are $\hbar\omega\big(n+\frac{1}{2}\big)$, $n = 0, 1, \dots$ (see Sect. 1.2). The single two-level system is defined by a self-adjoint operator acting in a two-dimensional complex Hilbert space and we denote by E_{g} and E_{e} its eigenvalues. We assume that the energy of the ground state E_{g} is less than the energy of the excited state E_{e}. The definition of the quantum Rabi Hamiltonian $\hat{H}_{\mathrm{Rabi}}$ uses the parameters

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ω, E_{g}, E_{e} and the coupling constant $g > 0$ present in the interaction term (see Sect. 1.4).

The main purpose of this paper is to describe a relation between the spectrum of the Hamiltonian $\hat{H}_{\mathrm{Rabi}}$ and the parameters used in its definition. It is well known that the spectrum of the quantum Rabi Hamiltonian is discrete and our main result is a three-term asymptotic formula describing the behavior of large eigenvalues. This formula involves all parameters of the model and allows us to determine the values of ω, E_{g}, E_{e}, g from the spectrum of $\hat{H}_{\mathrm{Rabi}}$.

The plan of the paper is the following. In Sect. 2 we state Theorem 2.1 describing our asymptotic formula. We also give references about related results. In Sect. 3 we give the main ideas of the proof of Theorem 2.1. Finally, in Sect. 4 we explain how to recover the values of all parameters, ω, E_{g}, E_{e}, and g from the asymptotic behavior of large eigenvalues of the quantum Rabi Hamiltonian.

1.2. The Hamiltonian of a single-mode quantized field

We fix $\omega > 0$ and a complex Hilbert space $\mathcal{H}_{\mathrm{field}}$ equipped with an orthonormal basis $\{\mathrm{e}_n\}_0^\infty$. We denote by $\hat{H}_{\mathrm{field}}$ the self-adjoint operator in $\mathcal{H}_{\mathrm{field}}$ given by

$$\hat{H}_{\mathrm{field}}\,\mathrm{e}_n = \hbar\omega\big(n + \tfrac{1}{2}\big)\mathrm{e}_n, \quad n = 0, 1, 2, \dots \tag{1.1}$$

1.3. The Hamiltonian of a two level quantum system

We introduce the level separation energy $E = E_{\mathrm{e}} - E_{\mathrm{g}} \geq 0$ and simplify the model choosing the zero energy so that the eigenvalues of the system are $\pm\frac{1}{2}E$. Taking $\mathcal{H}_{\mathrm{atom}} = \mathbb{C}^2$ and identifying e_{e}, e_{g} with the canonical basis of $\mathbb{C}^2$ we have

$$\hat{H}_{\mathrm{atom}} = \frac{1}{2}\,E\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}. \tag{1.2}$$

1.4. The quantum Rabi Hamiltonian

We define $\hat{H}_{\mathrm{Rabi}}$ as the self-adjoint operator in $\mathbb{C}^2 \otimes \mathcal{H}_{\mathrm{field}}$ given by the formula

$$\hat{H}_{\mathrm{Rabi}} = \hat{H}_{\mathrm{atom}} \otimes I_{\mathcal{H}_{\mathrm{field}}} + I_{\mathbb{C}^2} \otimes \hat{H}_{\mathrm{field}} + \hat{H}_{\mathrm{int}}, \tag{1.3}$$

where $\hat{H}_{\mathrm{int}}$ is an interaction term defined by

$$\hat{H}_{\mathrm{int}} = \hbar g\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix} \otimes (\hat{a} + \hat{a}^\dagger), \tag{1.4}$$

where $g > 0$ is the coupling constant, and $\hat{a}$ and $\hat{a}^\dagger$ are the photon annihilation and creation operators defined in $\mathcal{H}_{\mathrm{field}}$ by

$$\begin{aligned}\hat{a}\,\mathrm{e}_n &= \sqrt{n}\,\mathrm{e}_{n-1}, && n = 0, 1, 2, \dots,\\ \hat{a}^\dagger\mathrm{e}_n &= \sqrt{n+1}\,\mathrm{e}_{n+1}, && n = 0, 1, 2, \dots\end{aligned}$$

(with $\mathrm{e}_{-1} := 0$). Let us note the relations $[\hat{a}, \hat{a}^\dagger] = I$ and $\hat{a}^\dagger\hat{a} = \hat{N}$, where $\hat{N}$ is the photon number operator charaterized by $\hat{N}\mathrm{e}_n = n\,\mathrm{e}_n$.

2. Asymptotic behavior of large eigenvalues of $\hat{H}_{\text{Rabi}}$

2.1. Main result

We assume that $\omega > 0$, $E \geq 0$, $g > 0$ are fixed and denote

$$r_n := (-1)^n \frac{E \cos\left(\frac{4g}{\omega}\sqrt{n} - \frac{\pi}{4}\right)}{2\sqrt{2\pi g/\omega}} n^{-\frac{1}{4}}. \tag{2.1}$$

If $\hat{H}_{\text{Rabi}}$ is given by (1.3), then its spectrum $\sigma(\hat{H}_{\text{Rabi}})$ is discrete. Moreover, there is a canonical splitting $\mathbb{C}^2 \otimes \mathcal{H}_{\text{field}} = \mathcal{H}_+ \oplus \mathcal{H}_-$ which is $\hat{H}_{\text{Rabi}}$-invariant (see Section 3.1) and we denote by

$$E_0^+ \leq \cdots \leq E_n^+ \leq E_{n+1}^+ \leq \cdots \quad \text{and} \quad E_0^- \leq \cdots \leq E_n^- \leq E_{n+1}^- \leq \cdots$$

the eigenvalues of the restrictions of $\hat{H}_{\text{Rabi}}$ to $\mathcal{H}_+$ and $\mathcal{H}_-$, respectively, enumerated in nondecreasing order, counting multiplicities.

Theorem 2.1 (behavior of large eigenvalues of $\hat{H}_{\text{Rabi}}$). *Let $\hat{H}_{\text{Rabi}}$ be the quantum Rabi Hamiltonian given by* (1.3), *with parameters $\omega > 0$, $E \geq 0$, and $g > 0$. Then $\hat{H}_{\text{Rabi}}$ has discrete spectrum and its eigenvalues can be enumerated by couples (E_n^+, E_n^-) as specified above:*

$$\sigma(\hat{H}_{\text{Rabi}}) = \{E_n^+\}_0^\infty \cup \{E_n^-\}_0^\infty.$$

Moreover, for any $\varepsilon > 0$, the large n behavior of these eigenvalues is given by

$$E_n^\pm = \hbar\omega\left(n + \frac{1}{2}\right) - \frac{\hbar g^2}{\omega} \pm r_n + \mathrm{O}(n^{-\frac{1}{2}+\varepsilon}), \tag{2.2}$$

where r_n is defined by (2.1) *and* $\mathrm{O} = \mathrm{O}_\varepsilon$.

2.2. Comments

The large n behavior of the eigenvalues $E_n^\pm$ of $\hat{H}_{\text{Rabi}}$ was already investigated by Schmutz [17] by means of the Bogoliubov transformation (see Sect. 3.2). In the special case $E = 0$ the Bogoliubov transformation allows one to diagonalize $\hat{H}_{\text{Rabi}}$ and to express explicitly its eigenvalues:

$$E_n^+ = E_n^- = \hbar\omega\left(n + \frac{1}{2}\right) - \frac{\hbar g^2}{\omega}.$$

For arbitrary E the first proof of the two-term asymptotic formula was given by E.A. Tur [20] and the following improved estimate

$$E_n^\pm = \hbar\omega\left(n + \frac{1}{2}\right) - \frac{\hbar g^2}{\omega} + \mathrm{O}(n^{-\frac{1}{16}})$$

was then proved by E.A. Yanovich [21]. The approximation

$$E_n^\pm \approx \hbar\omega\left(n + \frac{1}{2}\right) - \frac{\hbar g^2}{\omega} \pm r_n$$

with r_n given by (2.1) was proposed on the basis of the 0th order approximation theory described by I.D. Feranchuk, L.I. Komarov, and A.P. Ulyanenkov in [8].

The same approximation was discovered independently by Irish [10]. Following Irish, it is called the Generalized Rotating Wave Approximation (GRWA) in the physical literature (see Sect. 3.2).

In Theorem 2.1 the remainder estimate $\mathrm{O}(n^{-\frac{1}{2}+\varepsilon})$ is uniform with respect to the coupling constant $g \in [C^{-1}, C]$ for any constant $C > 1$. On the other hand, for small values of g, perturbation theory gives expansions of $E_n^{\pm}$ in powers of g that provide information of a different nature, applicable only if ng^2 is small (see [9]).

We also mention that the method of successive diagonalizations was used in [1–3, 11, 13] to obtain the asymptotic behavior of large eigenvalues for similar models of infinite Jacobi matrices, but this approach does not apply to the quantum Rabi model (see also [4]).

Finally, we remark that the Rotating Wave Approximation (RWA) of the Jaynes–Cummings model gives an explicit expression for all eigenvalues that leads to an asymptotic behavior completely different from (2.2).

3. Main ingredients of the proof of Theorem 2.1

3.1. Reduction to Jacobi matrices

The first step of the proof consists in reducing the original problem to the analysis of Jacobi matrices J_α^β where α and $\beta > 0$ are real constants and

$$J_\alpha^\beta := \begin{pmatrix} \alpha & \beta\sqrt{1} & 0 & 0 & 0 & \dots \\ \beta\sqrt{1} & 1-\alpha & \beta\sqrt{2} & 0 & 0 & \dots \\ 0 & \beta\sqrt{2} & 2+\alpha & \beta\sqrt{3} & 0 & \dots \\ 0 & 0 & \beta\sqrt{3} & 3-\alpha & \beta\sqrt{4} & \dots \\ 0 & 0 & 0 & \beta\sqrt{4} & 4+\alpha & \dots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \ddots \end{pmatrix} \tag{3.1}$$

To describe this reduction we introduce $\{f_n^{\pm}\}_0^\infty$ by

$$f_{2k}^+ = \mathrm{e_e} \otimes \mathrm{e}_{2k}, \quad f_{2k+1}^+ = \mathrm{e_g} \otimes \mathrm{e}_{2k+1}, \quad f_{2k}^- = \mathrm{e_g} \otimes \mathrm{e}_{2k}, \quad f_{2k+1}^- = \mathrm{e_e} \otimes \mathrm{e}_{2k+1},$$

where $\{\mathrm{e_e}, \mathrm{e_g}\}$ and $\{\mathrm{e}_n\}_0^\infty$ are the canonical basis of $\mathcal{H}_{\mathrm{atom}} = \mathbb{C}^2$ and $\mathcal{H}_{\mathrm{field}}$, respectively. Denoting by $\mathcal{H}_+$ and $\mathcal{H}_-$ the closed subspaces generated by $\{f_n^+\}_0^\infty$ and $\{f_n^-\}_0^\infty$, respectively, we obtain

$$\mathbb{C}^2 \otimes \mathcal{H}_{\mathrm{field}} = \mathcal{H}_+ \oplus \mathcal{H}_-$$

and it can be easily checked (see, e.g., [19]) that the subspaces $\mathcal{H}_\pm$ are $\hat{H}_{\mathrm{Rabi}}$-invariant. Let $\hat{H}_{\mathrm{Rabi}}^{\pm}$ denote the restrictions of $\hat{H}_{\mathrm{Rabi}}$ to the subspaces $\mathcal{H}_\pm$. We then have the decomposition

$$\sigma(\hat{H}_{\mathrm{Rabi}}) = \sigma(\hat{H}_{\mathrm{Rabi}}^+) \cup \sigma(\hat{H}_{\mathrm{Rabi}}^-),$$

and thus it remains to investigate the eigenvalues $\{E_n^\pm\}_0^\infty$ of both operators $\hat{H}^\pm_{\mathrm{Rabi}}$. Finally, we consider the operators $\hat{H}_\pm$ defined by

$$\hat{H}^\pm_{\mathrm{Rabi}} = \tfrac{1}{2}\hbar\omega + \hbar\omega\hat{H}_\pm. \tag{3.2}$$

Their matrix elements in the basis $\{f_n^\pm\}_0^\infty$ form two Jacobi matrices J_α^β with $\alpha = \pm\frac{E}{2\hbar\omega}$ and $\beta = \frac{g}{\omega}$, i.e.,

$$\Big(\langle f_j^\pm|\hat{H}_\pm|f_k^\pm\rangle\Big)_{j,k=0}^\infty = J^{g/\omega}_{\pm E/(2\hbar\omega)}. \tag{3.3}$$

Let $\hat{J}_\alpha^\beta$ denote the self-adjoint operator defined by the matrix J_α^β in a complex Hilbert space $\mathcal{H}$ equipped with an orthonormal basis $\{\mathrm{e}_n\}_0^\infty$, i.e.,

$$\big(\langle \mathrm{e}_j|\hat{J}_\alpha^\beta|\mathrm{e}_k\rangle\big)_{j,k=0}^\infty = J_\alpha^\beta,$$

and let $\{\lambda_n^{\alpha,\beta}\}_{n=0}^\infty$ denote the sequence of eigenvalues of $\hat{J}_\alpha^\beta$, enumerated in non-decreasing order, counting multiplicities. Then $\hat{H}_\pm = \hat{J}^{g/\omega}_{\pm E/(2\hbar\omega)}$, and (2.2) follows from (3.2) and from

$$\lambda_n^{\alpha,\beta} = n - \beta^2 + \alpha(-1)^n \frac{\cos\big(4\beta\sqrt{n} - \frac{\pi}{4}\big)}{\sqrt{2\pi\beta\sqrt{n}}} + \mathrm{O}(n^{-\frac{1}{2}+\varepsilon}). \tag{3.4}$$

By (3.4) we indeed have

$$\begin{aligned}\lambda_n^{\pm\frac{E}{2\hbar\omega},\frac{g}{\omega}} &= n - \frac{g^2}{\omega^2} \pm (-1)^n \frac{E}{2\hbar\omega}\frac{\cos(4\frac{g}{\omega}\sqrt{n} - \frac{\pi}{4})}{\sqrt{2\pi g/\omega}}\, n^{-1/4} + \mathrm{O}(n^{-\frac{1}{2}+\varepsilon})\\ &= n - \frac{g^2}{\omega^2} \pm \frac{r_n}{\hbar\omega} + \mathrm{O}(n^{-\frac{1}{2}+\varepsilon}),\end{aligned}$$

hence, using (3.2),

$$E_n^\pm = \frac{1}{2}\hbar\omega + \hbar\omega\lambda_n^{\pm\frac{E}{2\hbar\omega},\frac{g}{\omega}} = \hbar\omega\left(n + \frac{1}{2}\right) - \frac{\hbar g^2}{\omega} \pm r_n + \mathrm{O}(n^{-\frac{1}{2}+\varepsilon}).$$

It remains to prove (3.4).

3.2. Bogoliubov transformation and GRWA

Using $\hat{N} = \hat{a}^\dagger\hat{a}$ (see Sect. 1.4), we can express $\hat{J}_\alpha^\beta$ as follows:

$$\hat{J}_\alpha^\beta = \hat{N} + \alpha\mathrm{e}^{\mathrm{i}\pi\hat{N}} + \beta(\hat{a} + \hat{a}^\dagger).$$

Moreover the spectrum of $\hat{J}_\alpha^\beta$ is the same as that of its Bogoliubov transform

$$\hat{G}_\alpha^\beta := \mathrm{e}^{\beta(\hat{a}^\dagger - \hat{a})}\,\hat{J}_\alpha^\beta\,\mathrm{e}^{-\beta(\hat{a}^\dagger - \hat{a})}.$$

For $\alpha = 0$ using that $[\hat{a}, \hat{a}^\dagger] = I$ we easily express the commutator $[\hat{a} - \hat{a}^\dagger, \hat{J}_0^\beta]$ as follows:

$$[\hat{a} - \hat{a}^\dagger, \hat{J}_0^\beta] = \hat{a} + \hat{a}^\dagger + 2\beta I. \tag{3.5}$$

This relation (3.5) allows us to get a simple expression of the derivative of $\hat{G}_0^\beta$ w.r.t. β:

$$\partial_\beta \hat{G}_0^\beta = \mathrm{e}^{\beta(\hat{a}^\dagger - \hat{a})} \left(\partial_\beta \hat{J}_0^\beta + [\hat{a}^\dagger - \hat{a}, \hat{J}_0^\beta] \right) \mathrm{e}^{-\beta(\hat{a}^\dagger - \hat{a})} = -2\beta I.$$

Thus,

$$\hat{G}_0^\beta = \hat{G}_0^0 - \beta^2 I = \hat{N} - \beta^2 I, \tag{3.6}$$

which implies that $\{n - \beta^2\}_{n=0}^\infty$ is the sequence of eigenvalues of $\hat{J}_0^\beta$.

Using (3.6) we then express $\hat{G}_\alpha^\beta$ as follows:

$$\hat{G}_\alpha^\beta = \hat{N} - \beta^2 I + \alpha \hat{V}_\beta, \tag{3.7}$$

where

$$\hat{V}_\beta := \mathrm{e}^{\beta(\hat{a}^\dagger - \hat{a})} \, \mathrm{e}^{\mathrm{i}\pi \hat{N}} \, \mathrm{e}^{-\beta(\hat{a}^\dagger - \hat{a})}. \tag{3.8}$$

According to Irish [10], the Generalized Rotating Wave Approximation consists in the approximation of $\lambda_n^{\alpha,\beta}$ by the diagonal entries of $\hat{G}_\alpha^\beta$. We claim (see Sect. 3.5) that this approximation holds modulo an error term $\mathrm{O}(n^{-1/2+\varepsilon})$, i.e., one has the large n estimate

$$\lambda_n^{\alpha,\beta} = \langle \mathrm{e}_n | \hat{G}_\alpha^\beta | \mathrm{e}_n \rangle + \mathrm{O}(n^{-1/2+\varepsilon}). \tag{GRWA}$$

In view of (3.7) we can write

$$\langle \mathrm{e}_n | \hat{G}_\alpha^\beta | \mathrm{e}_n \rangle = n - \beta^2 + \alpha \mathfrak{r}_\beta(n) \tag{3.9}$$

where $\mathfrak{r}_\beta(n)$ denotes the nth diagonal element of $\hat{V}_\beta$, i.e., $\mathfrak{r}_\beta(n) := \langle \mathrm{e}_n | \hat{V}_\beta | \mathrm{e}_n \rangle$. Then (3.4) follows from (GRWA) and from the estimate

$$\mathfrak{r}_\beta(n) = (-1)^n \frac{\cos\left(4\beta\sqrt{n} - \frac{\pi}{4}\right)}{\sqrt{2\pi\beta\sqrt{n}}} + \mathrm{O}(n^{-\frac{1}{2}} \ln n). \tag{3.10}$$

Thus it remains to prove (3.10) and (GRWA). The idea of the proof of (3.10) is given in Sect. 3.4 and a sketch of the proof of (GRWA) is given in Sect. 3.5.

3.3. Approximation of $\mathbf{e}^{t(\hat{a}^\dagger \quad \hat{a})}$

We introduce the function

$$\psi(t, j, \mathrm{e}^{\mathrm{i}\xi}) = 2t\sqrt{j} \sin\xi - t^2 \sin\xi \, \cos\xi, \tag{3.11}$$

where j is a nonnegative integer, t and ξ are real numbers. This function satisfies the large j estimate

$$\partial_t \psi(t, j, \mathrm{e}^{\mathrm{i}\xi}) + \sqrt{j} \, \mathrm{Im} \left(2\mathrm{e}^{\mathrm{i}(\psi(t,j+1,\mathrm{e}^{\mathrm{i}\xi}) - \psi(t,j,\mathrm{e}^{\mathrm{i}\xi}) - \xi)} \right) = \mathrm{O}(j^{-\frac{1}{2}}). \tag{3.12}$$

Following [5] we consider (3.12) as an approximative eiconal equation and prove that the operator $\hat{Q}_t$ defined by the relations

$$\langle \mathrm{e}_j | \hat{Q}_t | \mathrm{e}_k \rangle = \int_0^{2\pi} \mathrm{e}^{\mathrm{i}(k-j)\xi + \mathrm{i}\psi(t,j,\mathrm{e}^{\mathrm{i}\xi})} \, \frac{\mathrm{d}\xi}{2\pi}$$

satisfies the large n estimate

$$\| \Pi_{n/2}^{2n} \left(\mathrm{e}^{t(\hat{a}^\dagger - \hat{a})} - \hat{Q}_t \right) \Pi_{n/2}^{2n} \| = \mathrm{O}(n^{-\frac{1}{2}} \ln n), \tag{3.13}$$

where $\Pi_{n/2}^{2n}$ denotes the orthogonal projection on the subspace spanned by $\{\mathrm{e}_k\}_{n/2}^{2n}$.

3.4. Proof of (3.10)

We first observe that

$$(\hat{a}^\dagger - \hat{a})\mathrm{e}^{\mathrm{i}\pi\hat{N}}\mathrm{e}_n = (-1)^n(\hat{a}^\dagger - \hat{a})\mathrm{e}_n = -\mathrm{e}^{\mathrm{i}\pi\hat{N}}(\hat{a}^\dagger - \hat{a})\mathrm{e}_n,$$

so $\hat{a}^\dagger - \hat{a} = \mathrm{e}^{-\mathrm{i}\pi\hat{N}}(\hat{a} - \hat{a}^\dagger)\mathrm{e}^{\mathrm{i}\pi\hat{N}}$ and $\mathrm{e}^{-\beta(\hat{a}^\dagger - \hat{a})} = \mathrm{e}^{-\mathrm{i}\pi\hat{N}}\mathrm{e}^{\beta(\hat{a}^\dagger - \hat{a})}\mathrm{e}^{\mathrm{i}\pi\hat{N}}$. Thus, (3.8) gives

$$\hat{V}_\beta = \mathrm{e}^{\mathrm{i}\pi\hat{N}}\mathrm{e}^{-2\beta(\hat{a}^\dagger - \hat{a})},$$

which yields $\mathfrak{r}_\beta(n) = (-1)^n\langle \mathrm{e}_n|\mathrm{e}^{-2\beta(\hat{a}^\dagger - \hat{a})}|\mathrm{e}_n\rangle$. By approximating $\mathrm{e}^{-2\beta(\hat{a}^\dagger - \hat{a})}$ with $\hat{Q}_{-2\beta}$ and using the large n estimate (3.13), we obtain

$$\mathfrak{r}_\beta(n) = (-1)^n\langle \mathrm{e}_n|\hat{Q}_{-2\beta}|\mathrm{e}_n\rangle + \mathrm{O}(n^{-\frac{1}{2}}\ln n).$$

It remains to analyze the large n behavior of

$$\langle \mathrm{e}_n|\hat{Q}_{-2\beta}|\mathrm{e}_n\rangle = \int_0^{2\pi} \mathrm{e}^{-4\mathrm{i}\beta\sqrt{n}\sin\xi}\, b(-2\beta, \mathrm{e}^{\mathrm{i}\xi})\frac{\mathrm{d}\xi}{2\pi}\,, \tag{3.14}$$

where $b(-2\beta, \mathrm{e}^{\mathrm{i}\xi}) = \mathrm{e}^{-2\mathrm{i}\beta^2\sin 2\xi}$.

The phase function $\xi \to \sin\xi$ has two critical points $\xi = \pm\pi/2$. Since they are non-degenerated and $b(-2\beta, \mathrm{e}^{\pm\mathrm{i}\pi/2}) = 1$, the stationary phase formula yields the estimate

$$\langle \mathrm{e}_n|\hat{Q}_{-2\beta}|\mathrm{e}_n\rangle = \sum_{\kappa=\pm 1}\frac{\mathrm{e}^{\mathrm{i}\kappa(4\beta\sqrt{n}-\pi/4)}}{2\sqrt{2\pi\beta\sqrt{n}}} + \mathrm{O}(n^{-\frac{1}{2}}), \tag{3.15}$$

which gives (3.10).

3.5. Sketch of the proof of (GRWA)

We want to prove that the eigenvalues of $\hat{J}_\alpha^\beta$ have, for any $\varepsilon > 0$, the asymptotic behavior

$$\lambda_n^{\alpha,\beta} = n - \beta^2 + \alpha\mathfrak{r}_\beta(n) + \mathrm{O}(n^{-\frac{1}{2}+\varepsilon}), \quad n \to \infty. \tag{3.16}$$

Using the Tauberian approach from [5, Sect. 11], we deduce this asymptotic estimate from estimates

$$\sum_{m=0}^{\infty}\Big(\chi(\lambda_m^{\alpha,\beta} - n) - \chi(m - \beta^2 + \alpha\mathfrak{r}_\beta(m) - n)\Big) = \mathrm{O}(n^{-\frac{1}{2}+\varepsilon}), \tag{3.17}$$

where $\chi\colon \mathbb{R} \to \mathbb{C}$ is an arbitrary fast decaying function whose Fourier transform

$$\mathcal{F}(\chi)(t) := \int_{\mathbb{R}} \chi(\lambda)\mathrm{e}^{-\mathrm{i}t\lambda}\,\mathrm{d}\lambda$$

has compact support. We then observe that (3.17) can be viewed as a trace estimate. It may indeed be written as follows:

$$\sum_{k=0}^{\infty}\langle \mathrm{e}_k|\hat{K}_{\alpha,n}^{\beta,\chi}|\mathrm{e}_k\rangle = \mathrm{O}(n^{-\frac{1}{2}+\varepsilon}), \tag{3.18}$$

where $\hat{K}^{\beta,\chi}_{\alpha,n} := \chi(\hat{G}^{\beta}_{\alpha} - n) - \chi(\hat{N} - \beta^2 + \alpha\mathfrak{r}_{\beta}(\hat{N}) - n)$. The proof of the trace estimate (3.18) follows the idea of [5], which is based on the fact that the inverse Fourier transform allows us to express

$$\hat{K}^{\beta,\chi}_{\alpha,n} = \int_{\mathbb{R}} \mathcal{F}(\chi)(t) \left(\mathrm{e}^{\mathrm{i}t\hat{G}^{\beta}_{\alpha}} - \mathrm{e}^{\mathrm{i}t(\hat{N} - \beta^2 + \alpha\mathfrak{r}_{\beta}(\hat{N}))} \right) \mathrm{e}^{-\mathrm{i}tn} \, \frac{\mathrm{d}t}{2\pi}. \tag{3.19}$$

We then consider the time-dependent Hamiltonian

$$\hat{H}^{\beta}_{\alpha}(t) := \alpha \mathrm{e}^{-\mathrm{i}t\hat{N}} \hat{V}_{\beta} \mathrm{e}^{\mathrm{i}t\hat{N}}$$

and the associated evolution $t \to \hat{U}^{\beta}_{\alpha}(t)$ characterized by

$$-\mathrm{i}\partial_t \hat{U}^{\beta}_{\alpha}(t) = \hat{H}^{\beta}_{\alpha}(t)\hat{U}^{\beta}_{\alpha}(t), \qquad \hat{U}^{\beta}_{\alpha}(0) = I. \tag{3.20}$$

It then follows from (3.7) and (3.20) that $\mathrm{e}^{\mathrm{i}t\hat{G}^{\beta}_{\alpha}} = \mathrm{e}^{\mathrm{i}t(\hat{N} - \beta^2)} U^{\beta}_{\alpha}(t)$. Using this expression in (3.19), we get

$$\langle \mathrm{e}_k | \hat{K}^{\beta,\chi}_{\alpha,n} | \mathrm{e}_k \rangle = \int_{\mathbb{R}} \mathcal{F}(\chi)(t) \left(u^{\alpha,\beta}_k(t) - \mathrm{e}^{\mathrm{i}t\alpha\mathfrak{r}_{\beta}(k))} \right) \mathrm{e}^{\mathrm{i}t(k - \beta^2 - n)} \, \frac{\mathrm{d}t}{2\pi},$$

where $u^{\alpha,\beta}_k(t) := \langle \mathrm{e}_k | \hat{U}^{\beta}_{\alpha}(t) | \mathrm{e}_k \rangle$.

Let now $t_0 > 0$ be such that $\operatorname{supp} \mathcal{F}(\chi) \subset [-t_0, t_0]$. Reasoning as in [5, Sect. 6], we can deduce the trace estimate (3.18) from

$$\sup_{-t_0 \le t \le t_0} \sup_{|k-n| \le \sqrt{n}} \left| \partial_t u^{\alpha,\beta}_k(t) - \mathrm{i}\alpha\mathfrak{r}_{\beta}(k) \right| = \mathrm{O}(n^{-\frac{1-\varepsilon}{2}}). \tag{3.21}$$

To prove (3.21) we consider the Dyson expansion

$$\hat{U}^{\beta}_{\alpha}(t) - I = \mathrm{i} \int_0^t \hat{H}^{\beta}_{\alpha}(t_1) \mathrm{d}t_1 + \sum_{\nu=2}^{\infty} \mathrm{i}^{\nu} \int_0^t \mathrm{d}t_1 \cdots \int_0^{t_{\nu-1}} \hat{H}^{\beta}_{\alpha}(t_1) \cdots \hat{H}^{\beta}_{\alpha}(t_{\nu}) \mathrm{d}t_{\nu}. \tag{3.22}$$

Since $\langle \mathrm{e}_k | \hat{H}^{\beta}_{\alpha}(t_1) | \mathrm{e}_k \rangle = \alpha \langle \mathrm{e}_k | \hat{V}_{\beta} | \mathrm{e}_k \rangle = \alpha\mathfrak{r}_{\beta}(k)$, the kth diagonal element of the first term in the right hand side of (3.22) is equal to $\mathrm{i}t\alpha\mathfrak{r}_{\beta}(k)$. It remains to prove that the diagonal elements of the other terms in the right hand side of (3.22) give a contribution of order $\mathrm{O}(n^{-\frac{1}{2}+\frac{\varepsilon}{2}})$. These estimates are proven using approximations of these terms by oscillatory integrals of a form similar as the right-hand side of (3.14). Full details are given in [6, Sects. 4 and 7].

4. How the parameters can be recovered from the spectrum

The spectrum of $\hat{H}_{\mathrm{Rabi}}$ consists of couples (E^+_n, E^-_n), $n = 0, 1, \ldots$ satisfying the asymptotic formula (2.2). It is clear that the first parameter can be recovered by

$$\omega = \lim_{n \to \infty} \frac{E^{\pm}_n}{\hbar n}. \tag{4.1}$$

Next we introduce the spacing

$$\delta_n := |E^+_n - E^-_n| \tag{4.2}$$

and we are going to describe how the remaining parameters of the quantum Rabi model, i.e., g and E can be recovered from the asymptotic behavior of the sequence $\{\delta_n\}_0^\infty$.

We first observe that, for any $\varepsilon > 0$, the large n asymptotics (2.2) ensures

$$n^{1/4}\delta_n = \tilde{\alpha}|\mathfrak{p}_\beta(n)| + \mathrm{O}(n^{-\frac{1}{4}+\varepsilon}), \quad n \to \infty, \tag{4.3}$$

where

$$\beta := \frac{g}{\omega}, \tag{4.4}$$

$$\tilde{\alpha} := \frac{E}{2\sqrt{2\pi\beta}}, \tag{4.5}$$

$$\mathfrak{p}_\beta(n) := \cos\left(4\beta\sqrt{n} - \frac{\pi}{4}\right). \tag{4.6}$$

The sequence $\{4\beta\sqrt{n}\}_1^\infty$ is dense in $\mathbb{R}/2\pi\mathbb{Z}$ ($\beta \neq 0$). Then $\limsup\limits_{n\to\infty} \mathfrak{p}_\beta(n) = 1$, and hence

$$\tilde{\alpha} = \limsup_{n\to\infty} n^{\frac{1}{4}}\delta_n. \tag{4.7}$$

To get g and E, it remains to recover β from the sequence $\{\delta_n\}_0^\infty$. For this purpose, we first introduce

$$\mathcal{N} := \{n \in \mathbb{N} : 2n^{1/4}\delta_n \geq \tilde{\alpha}\}. \tag{4.8}$$

It follows from (4.3) that $\mathcal{N}$ is infinite and that for some integer n_0,

$$|\mathfrak{p}_\beta(n)| \geq \frac{1}{3} \quad \text{for any } n \in \mathcal{N},\ n \geq n_0. \tag{4.9}$$

In what follows we fix a real constant $\frac{3}{8} < \gamma < \frac{1}{2}$ and an auxiliary sequence of integers $\{k_n\}_0^\infty$, e.g., $k_n = \lfloor n^\gamma \rfloor$ such that

$$k_n = n^\gamma + \mathrm{O}(1), \quad n \to \infty. \tag{4.10}$$

If we consider

$$\mu_n := \frac{(n+k_n)^{1/4}\delta_{n+k_n} + (n-k_n)^{1/4}\delta_{n-k_n}}{2n^{1/4}\delta_n}, \tag{4.11}$$

then, due to (4.3), (4.8), and (4.9), we have

$$\mu_n = \frac{|\mathfrak{p}_\beta(n+k_n)| + |\mathfrak{p}_\beta(n-k_n)|}{2|\mathfrak{p}_\beta(n)|} + \mathrm{O}(n^{-\frac{1}{4}+\varepsilon}) \quad \text{for } n \in \mathcal{N},\ n \to \infty. \tag{4.12}$$

Using now $s = \pm k_n$ in

$$\sqrt{n+s} = \sqrt{n}\left(1 + \frac{s}{2n}\right) + \mathrm{O}(n^{-\frac{3}{2}}s^2), \quad n,\, s \to \infty, \tag{4.13}$$

and the assumption $\gamma < 1/2$, we find that $\mathfrak{p}_\beta(n \pm k_n) - \mathfrak{p}_\beta(n) \to 0$ as $n \to \infty$, hence $\mathfrak{p}_\beta(n \pm k_n)$ and $\mathfrak{p}_\beta(n)$ have the same sign for $n \in \mathcal{N}$ large enough. Thus (4.12) can also be written

$$\mu_n = \frac{\mathfrak{p}_\beta(n+k_n) + \mathfrak{p}_\beta(n-k_n)}{2\mathfrak{p}_\beta(n)} + \mathrm{O}(n^{-\frac{1}{4}+\varepsilon}) \quad \text{for } n \in \mathcal{N},\ n \to \infty. \tag{4.14}$$

Observe now that $\mathfrak{p}_\beta(n+k_n)+\mathfrak{p}_\beta(n-k_n)$ can be written as

$$2\cos\Big(2\beta(\sqrt{n+k_n}+\sqrt{n-k_n})-\frac{\pi}{4}\Big)\cos\Big(2\beta(\sqrt{n+k_n}-\sqrt{n-k_n})\Big). \tag{4.15}$$

Using again (4.13) with $s=\pm k_n$ and the asymptotics $n^{-\frac{3}{2}}k_n^2 \sim n^{-\frac{3}{2}+2\gamma}$, we can rewrite (4.15) as

$$2\left(\mathfrak{p}_\beta(n)+\mathrm{O}(n^{-\frac{3}{2}+2\gamma})\right)\left(\cos(2\beta n^{-1/2}k_n)+\mathrm{O}(n^{-\frac{3}{2}+2\gamma})\right), \quad n\to\infty. \tag{4.16}$$

Writing $\cos s = 1-\frac{1}{2}s^2+\mathrm{O}(s^4)$ in (4.16), as $n\to\infty$, we get

$$\mathfrak{p}_\beta(n+k_n)+\mathfrak{p}_\beta(n-k_n)=2\mathfrak{p}_\beta(n)\left(1-2\beta^2n^{-1}k_n^2+\mathrm{O}(n^{-2}k_n^4)\right)+\mathrm{O}(n^{-\frac{3}{2}+2\gamma}). \tag{4.17}$$

Combining (4.17) with (4.14), and using (4.9), we then obtain

$$\mu_n = 1-2\beta^2n^{-1}k_n^2+\mathrm{O}(n^{-2}k_n^4)+\mathrm{O}(n^{-\frac{3}{2}+2\gamma})+\mathrm{O}(n^{-\frac{1}{4}+\varepsilon}) \quad \text{for } n\in\mathcal{N},\ n\to\infty.$$

Since $\gamma<\frac{1}{2}$, we have $-\frac{3}{2}+2\gamma<-\frac{1}{4}+\varepsilon$ and the error term $\mathrm{O}(n^{-\frac{3}{2}+2\gamma})$ can be forgotten. Moreover, $n\,k_n^{-2}\,n^{-\frac{1}{4}+\varepsilon}\sim n^{\frac{3}{4}-2\gamma+\varepsilon}$, and we finally get

$$2\beta^2 = n\,k_n^{-2}(1-\mu_n)+\mathrm{O}(n^{-1}k_n^2)+\mathrm{O}(n^{\frac{3}{4}-2\gamma+\varepsilon}) \quad \text{for } n\in\mathcal{N},\ n\to\infty.$$

The first error term is o(1) since $n^{-1}k_n^2\sim n^{-1+2\gamma}$ with $\gamma<\frac{1}{2}$. The last error term is also o(1) provided $\varepsilon>0$ is small enough to have $\frac{3}{4}-2\gamma+\varepsilon<0$, which is possible by the hypothesis $\gamma>3/8$. We thus recover β from the spectrum by

$$2\beta^2=\lim_{\substack{n\in\mathcal{N}\\ n\to\infty}} n\,k_n^{-2}(1-\mu_n), \tag{4.18}$$

where $\mathcal{N}$ is given by (4.8), k_n by (4.10), and μ_n by (4.11). Due to (4.4) and (4.5), we can now recover the parameters g and E by using (4.18) with (4.1) and (4.7), respectively.

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Scattering theory for a class of non-selfadjoint extensions of symmetric operators

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To the fond memory of Professor Boris Pavlov

Abstract. This work deals with the functional model for a class of extensions of symmetric operators and its applications to the theory of wave scattering. In terms of Boris Pavlov's spectral form of this model, we find explicit formulae for the action of the unitary group of exponentials corresponding to *almost solvable* extensions of a given closed symmetric operator with equal deficiency indices. On the basis of these formulae, we are able to construct wave operators and derive a new representation for the scattering matrix for pairs of such extensions in both self-adjoint and non-self-adjoint situations.

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1. Introduction

Over the last 80 years or so, the subject of the mathematical analysis of waves interacting with obstacles and structures ('scattering theory') has served as one of the most impressive examples of bridging abstract mathematics and applications to physics, which in turn motivated the development of new mathematical techniques. The pioneering works of von Neumann [69, 70] and his contemporaries during 1930–1950, on the mathematical foundations of quantum mechanics, fuelled the interest of mathematical analysts to formulating and addressing the problems of direct and inverse wave scattering in a rigorous way.

The foundations of the modern mathematical scattering theory were laid by Friedrichs, Kato and Rosenblum [29, 71, 22] and subsequently by Birman and Kreĭn [5], Birman [4], Kato and Kuroda [30] and Pearson [54]. For a detailed exposition of this subject, see [55, 73].

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The direct and inverse scattering on the infinite and semi-infinite line was extensively studied using the classical integral-operator techniques by Borg [7, 8], Levinson [41], Krein [36, 37, 38], Gel'fand and Levitan [23], Marchenko [45], Faddeev [20, 21], Deift and Trubowitz [15]. In this body of work, the crucial role is played by the classical Weyl–Titchmarsh m-coefficient.

In the general operator-theoretic context, the m-coefficient is generalised to both the classical Dirichlet-to-Neumann map (in the PDE setting; cf. also [3]), and to the so-called M-operator, which takes the form of the Weyl–Titchmarsh M-matrix in the case of symmetric operators with equal deficiency indices. This has been exploited extensively in the study of operators, self-adjoint and non-selfadjoint alike, through the works in Ukraine (brought about by the influence of M. Kreĭn) on the theory of boundary triples and the associated M-operators (Gorbachuk and Gorbachuk [25], Kočubeĭ [32, 33], Derkach and Malamud [17] and further developments) and of the students of Pavlov in St. Petersburg (see e.g. [60, 31, 10]).

A parallel approach, which provides a connection to the theory of dissipative operators, was developed by Lax and Phillips [40], who analysed the direct scattering problem for a wide class of linear operators in the Hilbert space, including those associated with the multi-dimensional acoustic problem outside an obstacle, using the language of group theory (and, indeed, thereby developing the semi-group methods in operator theory). The associated techniques were also termed 'resonance scattering' by Lax and Phillips.

By virtue of the underlying dissipative framework, the above activity set the stage for the applications of non-selfadjoint techniques, in particular for the functional model for contractions and dissipative operators by Szökefalvi-Nagy and Foiaş [67], which has shown the special rôle in it of the characteristic function of Livšic [43] and allowed Pavlov [53] to construct a spectral form of the functional model for dissipative operators. The connection between this work and the concepts of scattering theory was uncovered by the famous theorem of Adamyan and Arov [1]. In a closely related development, Adamyan and Pavlov [2] established a description for the scattering matrix of a pair of self-adjoint extensions of a symmetric operator (densely or non-densely defined) with finite equal deficiency indices.

Further, Naboko [48] advanced the research initiated by Pavlov, Adamyan and Arov in two directions. Firstly, he generalised Pavlov's construction to the case of non-dissipative operators, and secondly, he provided explicit formulae for the wave operators and scattering matrices of a pair of (in general, non-selfadjoint) operators in the functional model setting. It is remarkable that in this work of Naboko the difference between the so-called stationary and non-stationary scattering approaches disappears.

There exists a wide body of work, carried out in the last 30 years or so, dedicated to the analysis of the scattering theory for general non-selfadjoint operators [44, 66, 68, 59, 63, 61]. These works make a substantial use of functional model techniques in the non-selfadjoint case and provide the most general results, without taking into account the specific features of any particular subclass of operators under consideration. In particular, the paper [63] essentially generalises to the non-selfadjoint case the classical stationary approach to the construction of wave operators [73]. On the other hand, as pointed out above, the study of non-selfadjoint extensions of symmetric operators naturally lends itself to the use of the theory of boundary triples and associated M-operators, thus taking advantage of the concrete properties of this subclass. This has been exploited in [60], where a functional model for dissipative and non-dissipative almost solvable extensions of symmetric operators was developed in terms of the theory of boundary triples. This work, however, stops short of the characterisation of the absolutely continuous subspace of the operator considered in the 'natural' terms associated with boundary triples and M-operators (cf. [59, 56], where the concept of the absolutely continuous subspace of a self-adjoint operator is discussed in the most general case). If one bridges this (in fact, very narrow) gap, as we do in Sections 3, 4, this opens up a possibility to directly apply Naboko's argument [48], which then yields both the explicit expression for wave operators and concise, easily checked sufficient conditions for the existence and completeness of wave operators, formulated in natural terms. What is more, it also yields an explicit expression for the scattering matrix of the problem, formulated in terms of the M-operator and parameters fixing the extension.

Our aim in the present work is therefore twofold: first, it is to expose the methodology of functional model in application to the development of scattering theory for non-selfadjoint operators and, second, to apply this methodology to the case of almost solvable extensions of symmetric operators, yielding new, concise and explicit, results in the special and important in applications case. With this aim in mind, we endeavour to extend the approach of Naboko [48], which was formulated for additive perturbations of self-adjoint operators, to the case of *both self-adjoint and non-self-adjoint* extensions of symmetric operators, under the only additional assumption that this extension is almost solvable, see Sect. 2 below for precise definitions. Unfortunately, the named assumption is rather restrictive in nature, see Remark 2 below. Still, already the framework of almost solvable extensions allows us to consider direct and inverse scattering problems on quantum graphs, see [14] for an application of abstract results of this paper in the mentioned setting. We also point out that the case we consider proves to be sufficiently generic to allow for a treatment of the scattering problem for models of double porosity in homogenisation, see [12, 13].

The paper is organised as follows. In Sect. 2 we recall the key points of the theory of boundary triples for extensions of symmetric operators with equal deficiency indices and introduce the associated M-operators, following mainly [17] and [60]. In Sect. 3 we derive formulae for the resolvents of the family of extensions $A_\varkappa$ parametrised by operators $\varkappa$ in the boundary space, in terms of the so-called characteristic function of a fixed element of the family. These formulae are then employed in Sect. 4 to derive the functional model for the above family of extensions. The material of Sects. 3 and 4 closely follows the approach of [60] and is based on the much more general facts of e.g. [48, 44, 59, 61], and references therein. Moreover, although this functional model can be seen as a particular case of more general results of the above papers, it proves however much more convenient for our purposes, due to the fact that it is explicitly formulated in the natural, from the point of view of the operator considered, terms. In Sect. 5 we characterise the absolutely continuous subspace of $A_\varkappa$ as the closure of the set of 'smooth' vectors in the model Hilbert space introduced in Sect. 4. In doing so, we follow the general framework of [59], but, again, the fact that we use the specifics of a particular class of non-selfadjoint operators allows us to obtain this characterisation in a concise, easily usable form. On this basis, in Sect. 6 we define the wave operators for a pair from the family $\{A_\varkappa\}$ and demonstrate their completeness property under natural, easily verifiable assumptions. This, in combination with the functional model, allows us to obtain formulae for the scattering operator of the pair. In Sect. 7 we describe the representation of the scattering operator as the scattering matrix, which is explicitly written in terms of the M-operator.

2. Extension theory and boundary triples

Let $\mathcal{H}$ be a separable Hilbert space and denote by $\langle\cdot,\cdot\rangle$ the inner product in this space.

Let A be a closed symmetric operator densely defined in $\mathcal{H}$, i.e. $A \subset A^*$, with domain $\operatorname{dom}(A) \subset \mathcal{H}$. The deficiency indices $n_+(A), n_-(A)$ are defined as follows:

$$n_\pm(A) := \dim(\mathcal{H} \ominus \operatorname{ran}(A - zI)) = \dim(\ker(A^* - \overline{z}I)), \quad z \in \mathbb{C}_\pm .$$

A closed operator L is said to be *completely non-selfadjoint* if there is no subspace reducing L such that the part of L in this subspace is self-adjoint. A completely non-selfadjoint symmetric operator is often referred to as *simple.*

As shown in [39, Sect. 1.3] (see also [26, Theorem 1.2.1]), the maximal invariant subspace for the closed symmetric operator A in which it is self-adjoint is $\bigcap_{z\in\mathbb{C}\setminus\mathbb{R}} \operatorname{ran}(A - zI)$. Thus, a necessary and sufficient condition for the closed symmetric operator A to be completely non-selfadjoint (or simple) is that

$$\bigcap_{z\in\mathbb{C}\setminus\mathbb{R}} \operatorname{ran}(A - zI) = \{0\} . \tag{1}$$

In this work we consider extensions of a given closed symmetric operator A with equal deficiency indices, i.e. $n_-(A) = n_+(A)$, and use the theory of boundary triples. In order to deal with the family of extensions $\{A_\varkappa\}$ of the symmetric operator A (where the parameter $\varkappa$ is itself an operator, see notation immediately following Proposition 2.2), we first construct a functional model of its particular dissipative extension. This is done following the Pavlov–Naboko procedure, which in turn stems from the functional model of Szökefalvi-Nagy and Foiaş. This allows us to obtain a simple model for the whole family $\{A_\varkappa\}$, in particular yielding a possibility to apply it to the scattering theory for certain pairs of operators in

$\{A_\varkappa\}$, for both cases when these operators are self-adjoint and non-selfadjoint, including the possibility that both operators of the pair are non-selfadjoint.

Taking into account the importance of dissipative operators in our work, we briefly recall that a densely defined operator L in $\mathcal{H}$ is called dissipative if

$$\operatorname{Im}\langle Lf, f\rangle \geq 0 \quad \forall f \in \operatorname{dom}(L). \tag{2}$$

A dissipative operator L is called maximal if $\mathbb{C}_-$ is contained in its resolvent set $\rho(L) := \{z \in \mathbb{C} : (L - zI)^{-1} \in \mathcal{B}(\mathcal{H})\}$ ($\mathcal{B}(\mathcal{H})$ denotes the space of bounded operators defined on the whole Hilbert space $\mathcal{H}$). Clearly, a maximal dissipative operator is closed; any dissipative operator admits a maximal extension.

We next describe the boundary triple approach to the extension theory of symmetric operators with equal deficiency indices (see [16] for a review of the subject). This approach has proven to be particularly useful in the study of self-adjoint extensions of ordinary differential operators of second order.

Definition 1. For a closed symmetric operator A with equal deficiency indices, consider the linear mappings

$$\Gamma_1 : \operatorname{dom}(A^*) \to \mathcal{K}, \quad \Gamma_0 : \operatorname{dom}(A^*) \to \mathcal{K},$$

where $\mathcal{K}$ is an auxiliary separable Hilbert space such that

$$(1) \quad \langle A^* f, g\rangle_{\mathcal{H}} - \langle f, A^* g\rangle_{\mathcal{H}} = \langle \Gamma_1 f, \Gamma_0 g\rangle_{\mathcal{K}} - \langle \Gamma_0 f, \Gamma_1 g\rangle_{\mathcal{K}}; \tag{3}$$

$$(2) \quad \text{The mapping } \operatorname{dom}(A^*) \ni f \mapsto \begin{pmatrix} \Gamma_1 f \\ \Gamma_0 f \end{pmatrix} \in \mathcal{K} \oplus \mathcal{K} \text{ is surjective.}$$

Then the triple $(\mathcal{K}, \Gamma_1, \Gamma_0)$ is said to be a *boundary triple* for A^*.

Remark 1. There exist boundary triples for A^* whenever A has equal deficiency indices (the case of infinite indices is not excluded), see [32, Theorem 3].

In this work we consider *proper extensions* of A, i.e. extensions of A that are restrictions of A^*. The extensions A_B for which there exists a triple $(\mathcal{K}, \Gamma_1, \Gamma_0)$ and $B \in \mathcal{B}(\mathcal{K})$ such that

$$f \in \operatorname{dom}(A_B) \iff \Gamma_1 f = B\Gamma_0 f\,. \tag{4}$$

are called *almost solvable* with respect to the triple $(\mathcal{K}, \Gamma_1, \Gamma_0)$.

Remark 2. Admittedly, the framework of almost solvable extensions is quite restrictive. In particular, even the standard three-dimensional scattering problem for PDEs in an exterior domain, with classical boundary condition (self-adjoint and non-selfadjoint alike) cannot be treated using this approach, see the discussion in [10] and also references therein. It would appear that one needs to employ the more general setting of linear relations [27], in order to accommodate this problem. However, the named setting is substantially more involved and complex than the theory of almost solvable extensions, so that the blueprints of the Sz-Nagy–Foiaş model of closed linear relations do not seem to be available as of today.

On the other hand, there exist at least two recent developments suggesting that the approach of the present paper can be extended beyond the natural limitations of the theory of almost solvable extensions. These are, firstly, the work [62], which offers a unified operator-theoretic approach to boundary-value problems and, in particular, an abstract definition of the M-operator suitable for the construction of a functional model; and secondly, the recent paper [11], which provides an explicit form of a functional model for PDE problems associated with dissipative operators. We hope to pursue this rather intriguing subject elsewhere.

The following assertions, written in slightly different terms, can be found in [32, Theorem 2] and [27, Chap. 3 Sect. 1.4] (see also [60, Theorem 1.1], and [64, Sect. 14] for an alternative formulation). We compile them in the next proposition for easy reference.

Proposition 2.1. *Let A be a closed symmetric operator with equal deficiency indices and let $(\mathcal{K}, \Gamma_1, \Gamma_0)$ be a the boundary triple for A^*. Assume that A_B is an almost solvable extension. Then the following statements hold:*

1. $f \in \operatorname{dom}(A)$ *if and only if* $\Gamma_1 f = \Gamma_0 f = 0$.
2. A_B *is maximal, i.e.* $\rho(A_B) \neq \emptyset$.
3. $A_B^* = A_{B^*}$.
4. A_B *is dissipative if and only if B is dissipative.*
5. A_B *is self-adjoint if and only if B is self-adjoint.*

Definition 2. The function $M : \mathbb{C}_- \cup \mathbb{C}_+ \to \mathcal{B}(\mathcal{H})$ such that

$$M(z)\Gamma_0 f = \Gamma_1 f \quad \forall f \in \ker(A^* - zI)$$

is *the Weyl function of the boundary triple* $(\mathcal{K}, \Gamma_1, \Gamma_0)$ for A^*, where A is assumed to be as in Proposition 2.1.

The Weyl function defined above has the following properties [17].

Proposition 2.2. *Let M be a Weyl function of the boundary triple $(\mathcal{K}, \Gamma_1, \Gamma_0)$ for A^*, where A is a closed symmetric operator with equal deficiency indices. Then the following statements hold:*

1. $M : \mathbb{C} \setminus \mathbb{R} \to \mathcal{B}(\mathcal{K})$.
2. M *is a $\mathcal{B}(\mathcal{K})$-valued double-sided $\mathcal{R}$-function* [28]*, that is,*

$$M(z)^* = M(\overline{z}) \qquad \text{and} \qquad \operatorname{Im}(z)\operatorname{Im}(M(z)) > 0 \quad \text{for } z \in \mathbb{C} \setminus \mathbb{R}\,.$$

3. *The spectrum of A_B coincides with the set of points $z_0 \in \mathbb{C}$ such that $(M - B)^{-1}$ does not admit analytic continuation into z_0.*

Let us lay out the notation for some of the main objects in this paper. In the auxiliary Hilbert space $\mathcal{K}$, choose a bounded nonnegative self-adjoint operator α so that the operator

$$B_\varkappa := \frac{\alpha\varkappa\alpha}{2} \tag{5}$$

belongs to $\mathcal{B}(\mathcal{K})$, where $\varkappa$ is a bounded operator in $E := \operatorname{clos}(\operatorname{ran}(\alpha)) \subset \mathcal{K}$. In what follows, we deal with almost solvable extensions of a given symmetric operator A

that are generated by $B_\varkappa$ via (4). We always assume that the deficiency indices of A are equal and that some boundary triple $(\mathcal{K}, \Gamma_1, \Gamma_0)$ for A^* is fixed. In order to streamline the formulae, we write

$$A_\varkappa := A_{B_\varkappa}. \tag{6}$$

Here $\varkappa$ should be understood as a parameter for a family of almost solvable extensions of A. Note that if $\varkappa$ is self-adjoint then so is $B_\varkappa$ and, hence by Proposition 2.1(5), $A_\varkappa$ is self-adjoint. Note also that $A_{\mathrm{i}I}$ is maximal dissipative, again by Proposition 2.1.

Definition 3. The characteristic function of the operator $A_{\mathrm{i}I}$ is the operator-valued function S on $\mathbb{C}_+$ given by

$$S(z) := I\restriction_E + \mathrm{i}\alpha\big(B_{\mathrm{i}I}^* - M(z)\big)^{-1}\alpha\restriction_E, \qquad z \in \mathbb{C}_+. \tag{7}$$

By [60, Eq. (1.16)], the above definition is a particular case of the so-called Štraus characteristic function, see [60, Definition 1.7].

Remark 3. The function S is analytic in $\mathbb{C}_+$ and, for each $z \in \mathbb{C}_+$, the mapping $S(z) : E \to E$ is a contraction. Therefore, S has nontangential limits almost everywhere on the real line in the strong topology [67], which we will henceforth denote by $S(k)$, $k \in \mathbb{R}$.

Remark 4. When $\alpha = \sqrt{2}I$, an straightforward calculation yields that $S(z)$ is the Cayley transform of $M(z)$, i.e.

$$S(z) = (M(z) - \mathrm{i}I)(M(z) + \mathrm{i}I)^{-1}.$$

3. Formulae for the resolvents of almost solvable extensions

In this section we establish some useful relations between the resolvents of the operators $A_\varkappa$ for any $\varkappa \in \mathcal{B}(E)$ and the resolvents of the maximal dissipative operator $A_{\mathrm{i}I}$ and its adjoint. These relations (cf. [63, 59, 61] and references therein, for the corresponding results in the general setting of closed non-selfadjoint operators) are instrumental for the construction of the functional model in the next section.

Notation 1. We abbreviate

$$\Theta_\varkappa(z) := I - \mathrm{i}\alpha(B_{\mathrm{i}I} - M(z))^{-1}\alpha\chi_\varkappa^+, \quad z \in \mathbb{C}_-, \tag{8}$$

$$\widehat{\Theta}_\varkappa(z) := I + \mathrm{i}\alpha(B_{\mathrm{i}I}^* - M(z))^{-1}\alpha\chi_\varkappa^-, \quad z \in \mathbb{C}_+, \tag{9}$$

where

$$\chi_\varkappa^\pm := \frac{I \pm \mathrm{i}\varkappa}{2}, \tag{10}$$

and for simplicity we have written I instead of $I\restriction_E$. We use this convention throughout the text.

It follows from Definition 3 and Proposition 2.2(2) that the operator-valued functions $\Theta_\varkappa(z)$ and $\widehat{\Theta}_\varkappa(z)$ can be expressed in terms of the characteristic function S, as follows:

$$\Theta_\varkappa(z) = I + (S^*(\overline{z}) - I)\chi_\varkappa^+ \quad \forall\, z \in \mathbb{C}_-\,, \tag{11}$$

$$\widehat{\Theta}_\varkappa(z) = I + (S(z) - I)\chi_\varkappa^- \quad \forall\, z \in \mathbb{C}_+\,. \tag{12}$$

The formulae in the next lemma are analogous to [60, Eqs. (2.18) and (2.22)].

Lemma 3.1. *The following identities hold:*

(i) $\alpha\Gamma_0(A_{\mathrm{i}I} - zI)^{-1} = \Theta_\varkappa(z)\alpha\Gamma_0(A_\varkappa - zI)^{-1} \quad \forall\, z \in \mathbb{C}_- \cap \rho(A_\varkappa)$*;*
(ii) $\alpha\Gamma_0(A_\varkappa - zI)^{-1} = \Theta_\varkappa(z)^{-1}\alpha\Gamma_0(A_{\mathrm{i}I} - zI)^{-1} \quad \forall\, z \in \mathbb{C}_- \cap \rho(A_\varkappa)$*;*
(iii) $\alpha\Gamma_0(A_{\mathrm{i}I}^* - zI)^{-1} = \widehat{\Theta}_\varkappa(z)\alpha\Gamma_0(A_\varkappa - zI)^{-1} \quad \forall\, z \in \mathbb{C}_+ \cap \rho(A_\varkappa)$*;*
(iv) $\alpha\Gamma_0(A_\varkappa - zI)^{-1} = \widehat{\Theta}_\varkappa(z)^{-1}\alpha\Gamma_0(A_{\mathrm{i}I}^* - zI)^{-1} \quad \forall\, z \in \mathbb{C}_+ \cap \rho(A_\varkappa)\,.$

Proof. We start by proving (i). To this end, suppose that $z \in \mathbb{C}_- \cap \rho(A_\varkappa)$ so $(A_{\mathrm{i}I} - zI)^{-1}$ and $(A_\varkappa - zI)^{-1}$ are defined on the whole space $\mathcal{H}$. Fix an arbitrary $h \in \mathcal{H}$ and define

$$\varphi := (A_{\mathrm{i}I} - zI)^{-1}h, \quad g := (A_\varkappa - zI)^{-1}h\,. \tag{13}$$

Clearly, the vector

$$f := \varphi - g = \left((A_{\mathrm{i}I} - zI)^{-1} - (A_\varkappa - zI)^{-1}\right) h$$

is in $\ker(A^* - zI)$ since A^* is an extension of both operators $A_{\mathrm{i}I}$ and $A_\varkappa$. According to (4), it follows from $\varphi \in \mathrm{dom}(A_{\mathrm{i}I})$ and $g \in \mathrm{dom}(A_\varkappa)$ that $\Gamma_1\varphi = B_{\mathrm{i}I}\Gamma_0\varphi$ and $\Gamma_1 g = B_\varkappa\Gamma_0 g$. Thus, one has

$$\begin{aligned} 0 &= \Gamma_1(f+g) - B_{\mathrm{i}I}\Gamma_0(f+g) \\ &= \Gamma_1 f - B_{\mathrm{i}I}\Gamma_0 f + \Gamma_1 g - B_{\mathrm{i}I}\Gamma_0 g \\ &= M(z)\Gamma_0 f - B_{\mathrm{i}I}\Gamma_0 f + B_\varkappa\Gamma_0 g - B_{\mathrm{i}I}\Gamma_0 g\,, \end{aligned}$$

where in the last equality we also use the fact that $f \in \ker(A^* - zI)$, together with Definition 2. Hence one has

$$\Gamma_0 f = (B_{\mathrm{i}I} - M(z))^{-1}(B_\varkappa - B_{\mathrm{i}I})\Gamma_0 g\,,$$

which, in turn, implies that

$$\Gamma_0\varphi = \Gamma_0 f + \Gamma_0 g = \left[I + (B_{\mathrm{i}I} - M(z))^{-1}(B_\varkappa - B_{\mathrm{i}I})\right]\Gamma_0 g. \tag{14}$$

Taking into account (13), using the fact that $B_\varkappa - B_{\mathrm{i}I} = -\mathrm{i}\alpha\chi_\varkappa^+\alpha$ and applying the operator α to both sides of (14), we obtain

$$\alpha\Gamma_0(A_{\mathrm{i}I} - zI)^{-1}h = \left[I - \mathrm{i}\alpha(B_{\mathrm{i}I} - M(z))^{-1}\alpha\chi_\varkappa^+\right]\alpha\Gamma_0(A_\varkappa - zI)^{-1}h,$$

which is the identity (i), in view of the definition (11).

Similar computations with the pairs $A_\varkappa, B_\varkappa$ and $A_{\mathrm{i}I}, B_{\mathrm{i}I}$ interchanged lead to

$$\alpha\Gamma_0(A_\varkappa - zI)^{-1}h = \left[I + \mathrm{i}\alpha(B_\varkappa - M(z))^{-1}\alpha\chi_\varkappa^+\right]\alpha\Gamma_0(A_{\mathrm{i}I} - zI)^{-1}h, \tag{15}$$

for $z \in \mathbb{C}_- \cap \rho(A_\varkappa)$. Now, (ii) follows from (15) using the identity

$$\Theta_\varkappa(z)^{-1} = I + \mathrm{i}\alpha\big(B_\varkappa - M(z)\big)^{-1}\alpha\chi_\varkappa^+ \quad \forall\, z \in \mathbb{C}_- \cap \rho(A_\varkappa)\,, \tag{16}$$

which is validated by multiplying together the right-hand sides of (16) and (8) and employing a version of the second resolvent identity (cf. [72, Theorem 5.13]):

$$(B_\varkappa - M(z))^{-1} - (B_{\mathrm{i}I} - M(z))^{-1} = (B_\varkappa - M(z))^{-1}(B_{\mathrm{i}I} - B_\varkappa)(B_{\mathrm{i}I} - M(z))^{-1}$$

which holds for all $z \in \mathbb{C}_- \cap \rho(A_\varkappa)$.

We next proceed to the proof of (iii) and (iv). Fix an arbitrary $z \in \mathbb{C}_+ \cap \rho(A_\varkappa)$ and an arbitrary $h \in \mathcal{H}$ and define

$$\varphi := (A_{\mathrm{i}I}^* - zI)^{-1}h\,, \quad g := (A_\varkappa - zI)^{-1}h\,, \tag{17}$$

then $f := \varphi - g$ is in $\ker(A^* - zI)$. Since $\varphi \in \operatorname{dom}(A_{\mathrm{i}I}^*)$, one has that

$$\begin{aligned} 0 &= \Gamma_1(f+g) - B_{\mathrm{i}I}^*\Gamma_0(f+g) \\ &= M(z)\Gamma_0 f + \Gamma_1 g - B_{\mathrm{i}I}^*\Gamma_0 f - B_{\mathrm{i}I}\Gamma_0 g\,, \end{aligned}$$

where in the second equality we use the fact that $f \in \ker(A^* - zI)$. On the other hand, in view of the inclusion $g \in \operatorname{dom}(A_\varkappa)$, the formula (4) allows us to replace the second term in the last expression by $B_\varkappa\Gamma_0 g$, which yields

$$0 = (M(z) - B_{\mathrm{i}I}^*)\Gamma_0 f + (B_\varkappa - B_{\mathrm{i}I}^*)\Gamma_0 g\,. \tag{18}$$

Since $B_\varkappa - B_{\mathrm{i}I}^* = \mathrm{i}\alpha\chi_\varkappa^-\alpha$, equality (18) is rewritten as

$$\Gamma_0 f = \mathrm{i}(B_{\mathrm{i}I}^* - M(z))^{-1}\alpha\chi_\varkappa^-\alpha\Gamma_0 g\,,$$

which in turn implies that

$$\Gamma_0\varphi = \left[I + \mathrm{i}(B_{\mathrm{i}I}^* - M(z))^{-1}\alpha\chi_\varkappa^-\alpha\right]\Gamma_0 g\,.$$

Applying the operator α to both sides of the last equation and using (17), we obtain

$$\alpha\Gamma_0(A_{\mathrm{i}I}^* - zI)^{-1}h = \left[I + \mathrm{i}\alpha(B_{\mathrm{i}I}^* - M(z))^{-1}\alpha\chi_\varkappa^-\right]\alpha\Gamma_0(A_\varkappa - zI)^{-1}h,$$

which is (iii), in view of the definition (12).

Finally, we interchange the operators $A_{\mathrm{i}I}^*$ and $A_\varkappa$ in (17) and repeat the computations, correspondingly interchanging $B_{\mathrm{i}I}$ and $B_\varkappa$. This yields the identity

$$\alpha\Gamma_0(A_\varkappa^* - zI)^{-1}h = \left[I - \mathrm{i}\alpha(B_{\mathrm{i}I}^* - M(z))^{-1}\alpha\chi_\varkappa^-\right]\alpha\Gamma_0(A_{\mathrm{i}I}^* - zI)^{-1}h, \tag{19}$$

for all $z \in \mathbb{C}_+ \cap \rho(A_\varkappa)$. In a similar way to (16), we verify that

$$\widehat{\Theta}_\varkappa(z)^{-1} = I - \mathrm{i}\alpha(B_{\mathrm{i}I}^* - M(z))^{-1}\alpha\chi_\varkappa^- \quad \forall\, z \in \mathbb{C}_+ \cap \rho(A_\varkappa)$$

and hence establish (iv). □

4. Functional model and theorems about smooth vectors

Following [48], we introduce a Hilbert space serving as a functional model for the family of operators $A_\varkappa$. This functional model was constructed for completely non-selfadjoint maximal dissipative operators in [53, 51, 52] and further developed in [48, 61, 59, 68]. Next we recall some related necessary information. In what follows, in various formulae, we use the subscript '±' to indicate two different versions of the same formula in which the subscripts '+' and '−' are taken individually.

A function f analytic on $\mathbb{C}_\pm$ and taking values in E is said to be in the Hardy class $H^2_\pm(E)$ when

$$\sup_{y>0}\int_{\mathbb{R}} \|f(x \pm \mathrm{i}y)\|^2_E \, dx < +\infty$$

(cf. [57, Sect. 4.8]). Whenever $f \in H^2_\pm(E)$, the left-hand side of the above inequality defines $\|f\|^2_{H^2_\pm(E)}$. We use the notation H^2_+ and H^2_- for the usual Hardy spaces of $\mathbb{C}$-valued functions.

The elements of the Hardy spaces $H^2_\pm(E)$ are identified with their boundary values, which exist almost everywhere on the real line. We keep the same notation $H^2_\pm(E)$ for the corresponding subspaces of $L^2(\mathbb{R}, E)$ [57, Sect. 4.8, Theorem B]). By the Paley–Wiener theorem [57, Sect. 4.8, Theorem E]), one verifies that these subspaces are the orthogonal complements of each other.

Following the argument of [48, Theorem 1], it is shown in [60, Lemma 2.4] that

$$\alpha\Gamma_0(A_{\mathrm{i}I} - \cdot I)^{-1}h \in H^2_-(E) \quad \text{and} \quad \alpha\Gamma_0(A^*_{\mathrm{i}I} - \cdot I)^{-1}h \in H^2_+(E)\,. \tag{20}$$

As mentioned in Remark 3, the characteristic function S given in Definition 3 has nontangential limits almost everywhere on the real line in the strong topology. Thus, for a two-component vector function $\binom{\widetilde{g}}{g}$ taking values in $E \oplus E$, one can consider the integral

$$\int_{\mathbb{R}} \left\langle \begin{pmatrix} I & S^*(s) \\ S(s) & I \end{pmatrix} \begin{pmatrix} \widetilde{g}(s) \\ g(s) \end{pmatrix}, \begin{pmatrix} \widetilde{g}(s) \\ g(s) \end{pmatrix} \right\rangle_{E\oplus E} ds, \tag{21}$$

which is always nonnegative, due to the contractive properties of S. The space

$$\mathfrak{H} := L^2\left(E \oplus E; \begin{pmatrix} I & S^* \\ S & I \end{pmatrix}\right) \tag{22}$$

is the completion of the linear set of two-component vector functions $\binom{\widetilde{g}}{g} : \mathbb{R} \to E \oplus E$ in the norm (21), factored with respect to vectors of zero norm. Naturally, not every element of the set can be identified with a pair $\binom{\widetilde{g}}{g}$ of two independent functions. Still, in what follows we keep the notation $\binom{\widetilde{g}}{g}$ for the elements of this space.

Another consequence of the contractive properties of the characteristic function S is that for $\widetilde{g}, g \in L^2(\mathbb{R}, E)$ one has

$$\left\| \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} \right\|_{\mathfrak{H}} \geq \begin{cases} \|\widetilde{g} + S^* g\|_{L^2(\mathbb{R},E)} , \\ \|S\widetilde{g} + g\|_{L^2(\mathbb{R},E)} . \end{cases}$$

Thus, for every Cauchy sequence $\{\binom{\widetilde{g}_n}{g_n}\}_{n=1}^{\infty}$, with respect to the $\mathfrak{H}$-topology, such that $\widetilde{g}_n, g_n \in L^2(\mathbb{R}, E)$ for all $n \in \mathbb{N}$, the limits of $\widetilde{g}_n + S^* g_n$ and $S\widetilde{g}_n + g_n$ exist in $L^2(\mathbb{R}, E)$, so that $\widetilde{g} + S^* g$ and $S\widetilde{g} + g$ can always be treated as $L^2(\mathbb{R}, E)$ functions.

Consider the orthogonal subspaces of $\mathfrak{H}$

$$D_- := \begin{pmatrix} 0 \\ H^2_-(E) \end{pmatrix} , \quad D_+ := \begin{pmatrix} H^2_+(E) \\ 0 \end{pmatrix} . \tag{23}$$

We define the space

$$K := \mathfrak{H} \ominus (D_- \oplus D_+),$$

which is characterised as follows (see e.g. [51, 52]):

$$K = \left\{ \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} \in \mathfrak{H} : \widetilde{g} + S^* g \in H^2_-(E) \, , S\widetilde{g} + g \in H^2_+(E) \right\} . \tag{24}$$

The orthogonal projection P_K onto the subspace K is given by (see e.g. [47])

$$P_K \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} = \begin{pmatrix} \widetilde{g} - P_+(\widetilde{g} + S^* g) \\ g - P_-(S\,\widetilde{g} + g) \end{pmatrix} , \tag{25}$$

where $P_\pm$ are the orthogonal Riesz projections in $L^2(E)$ onto $H^2_\pm(E)$.

A completely non-selfadjoint dissipative operator admits [67] a self-adjoint dilation. The dilation $\mathcal{A} = \mathcal{A}^*$ of the operator $A_{\mathrm{i}I}$ is constructed following Pavlov's procedure [51, 53, 52]: it is defined in the Hilbert space

$$\mathscr{H} = L^2(\mathbb{R}_-, \mathcal{K}) \oplus \mathcal{H} \oplus L^2(\mathbb{R}_+, \mathcal{K}), \tag{26}$$

so that

$$P_{\mathcal{H}}(\mathcal{A} - zI)^{-1} \upharpoonright_{\mathcal{H}} = (A_{\mathrm{i}I} - zI)^{-1} , \quad z \in \mathbb{C}_- .$$

As in the case of additive non-selfadjoint perturbations [48], Ryzhov established in [60, Theorem 2.3] that $\mathfrak{H}$ serves as the functional model for the dilation $\mathcal{A}$, i.e. there exists an isometry $\Phi : \mathscr{H} \to \mathfrak{H}$, which we will make explicit below in our particular setting, such that $\mathcal{A}$ is transformed into the operator of multiplication by the independent variable, $\Phi(\mathcal{A} - zI)^{-1} = (\cdot - z)^{-1}\Phi$. Furthermore, under this isometry

$$\Phi \upharpoonright_{\mathcal{H}} \mathcal{H} = K$$

unitarily, where $\mathcal{H}$ is understood as being embedded in $\mathscr{H}$ in the natural way, i.e.

$$\mathcal{H} \ni h \mapsto 0 \oplus h \oplus 0 \in \mathscr{H}.$$

In what follows we keep the label Φ for the restriction $\Phi \upharpoonright_{\mathcal{H}}$, hoping that it does not lead to confusion.

The next theorem generalises [60, Theorem 2.5], and its form is similar to [48, Theorem 3], which treats the case of additive perturbations, see also [44, 60, 59, 61] for the case of possibly non-additive perturbations. The proof blends together the arguments of [60] and [48], taking advantage of the similarity between the formulae (8)–(12) and those of [48, Sect. 2]. It is standard, see e.g. [44, 48, 61], and is therefore included in the Appendix for the sake of completeness only.

Theorem 4.1. *(i) If $z \in \mathbb{C}_- \cap \rho(A_\varkappa)$ and $\binom{\widetilde{g}}{g} \in K$, then*

$$\Phi(A_\varkappa - zI)^{-1}\Phi^* \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} = P_K \frac{1}{\cdot - z} \begin{pmatrix} \widetilde{g} \\ g - \chi_\varkappa^+ \Theta_\varkappa^{-1}(z)(\widetilde{g} + S^* g)(z) \end{pmatrix}. \tag{27}$$

(ii) If $z \in \mathbb{C}_+ \cap \rho(A_\varkappa)$ and $\binom{\widetilde{g}}{g} \in K$, then

$$\Phi(A_\varkappa - zI)^{-1}\Phi^* \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} = P_K \frac{1}{\cdot - z} \begin{pmatrix} \widetilde{g} - \chi_\varkappa^- \widehat{\Theta}_\varkappa^{-1}(z)(S\widetilde{g} + g)(z) \\ g \end{pmatrix}. \tag{28}$$

Here, $(\widetilde{g} + S^* g)(z)$ and $(S\widetilde{g} + g)(z)$ denote the values at z of the analytic continuations of the functions $\widetilde{g} + S^* g \in H^2_-(E)$ and $S\widetilde{g} + g \in H^2_+(E)$ into the lower half-plane and upper half-plane, respectively.

Following the ideas of Naboko, in the functional model space $\mathfrak{H}$ consider two subspaces $\mathfrak{N}_\pm^\varkappa$ defined as follows:

$$\mathfrak{N}_\pm^\varkappa := \left\{ \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} \in \mathfrak{H} : P_\pm \left(\chi_\varkappa^+ (\widetilde{g} + S^* g) + \chi_\varkappa^- (S\widetilde{g} + g) \right) = 0 \right\}. \tag{29}$$

These subspaces have a characterisation in terms of the resolvent of the operator $A_\varkappa$. This, again, can be seen as a consequence of a much more general argument (see e.g. [61, 59]). The proof in our particular case is provided in Appendix and follows the approach of [48, Theorem 4].

Theorem 4.2. *Suppose that* $\ker\{\alpha\} = 0$. *The following characterisation holds:*

$$\mathfrak{N}_\pm^\varkappa = \left\{ \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} \in \mathfrak{H} : \Phi(A_\varkappa - zI)^{-1}\Phi^* P_K \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} = P_K \frac{1}{\cdot - z} \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} \text{ for all } z \in \mathbb{C}_\pm \right\}. \tag{30}$$

Consider the counterparts of $\mathfrak{N}_\pm^\varkappa$ in the original Hilbert space $\mathcal{H}$:

$$\widetilde{N}_\pm^\varkappa := \Phi^* P_K \mathfrak{N}_\pm^\varkappa, \tag{31}$$

which are linear sets albeit not necessarily subspaces. In a way similar to [48], we introduce the set

$$\widetilde{N}_{\mathrm{e}}^\varkappa := \widetilde{N}_+^\varkappa \cap \widetilde{N}_-^\varkappa$$

of so-called smooth vectors and its closure $N_{\mathrm{e}}^\varkappa := \operatorname{clos}(\widetilde{N}_{\mathrm{e}}^\varkappa)$. In Sect. 5 we prove that $N_{\mathrm{e}}^\varkappa$ coincides with the absolutely continuous subspace of the operator $A_\varkappa$ in the case when $A_\varkappa = A_\varkappa^*$ and under the additional assumption that $\ker(\alpha) = \{0\}$, as in Theorem 4.2.

The next assertion (cf. e.g. [61, 59], for the case of general non-selfadjoint operators), whose proof is found in Appendix, is an alternative non-model characterisation of the linear sets $\widetilde{N}_\pm^\varkappa$.

Theorem 4.3. *The sets* $\widetilde{N}_\pm^\varkappa$ *are described as follows:*

$$\widetilde{N}_\pm^\varkappa = \left\{u \in \mathcal{H} : \chi_\varkappa^\mp \alpha\Gamma_0(A_\varkappa - zI)^{-1}u \in H_\pm^2(E)\right\}. \tag{32}$$

Corollary 4.4. *The right-hand side of* (32) *coincides with* $\{u \in \mathcal{H} : \alpha\Gamma_0(A_\varkappa - zI)^{-1}u \in H_\pm^2(E)\}$, *and therefore equivalently one has*

$$\widetilde{N}_\pm^\varkappa = \{u \in \mathcal{H} : \alpha\Gamma_0(A_\varkappa - zI)^{-1}u \in H_\pm^2(E)\}. \tag{33}$$

Proof. Indeed, if $\alpha\Gamma_0(A_\varkappa - zI)^{-1}u \in H_+^2(E)$ then clearly $\chi_\varkappa^-\alpha\Gamma_0(A_\varkappa - zI)^{-1}u \in H_+^2(E)$. Conversely, we write

$$\begin{aligned} S(z)\chi_\varkappa^-\alpha\Gamma_0(A_\varkappa - zI)^{-1}u & \\ &= (S(z)\chi_\varkappa^- + \chi_\varkappa^+)\alpha\Gamma_0(A_\varkappa - zI)^{-1}u - \chi_\varkappa^+\alpha\Gamma_0(A_\varkappa - zI)^{-1}u \quad (34)\\ &= \widehat{\Theta}_\varkappa(z)\alpha\Gamma_0(A_\varkappa - zI)^{-1}u - \chi_\varkappa^+\alpha\Gamma_0(A_\varkappa - zI)^{-1}u \quad (35)\\ &= \alpha\Gamma_0(A_{iI}^* - zI)^{-1}u - \chi_\varkappa^+\alpha\Gamma_0(A_\varkappa - zI)^{-1}u, \quad (36)\end{aligned}$$

where $S(z)\chi_\varkappa^- + \chi_\varkappa^+ = (S(z) - I)\chi_\varkappa^- + I = \widehat{\Theta}_\varkappa(z)$, see (12), and in (35)–(36) we use the part (iii) of Lemma 3.1.

Further, as we noted in (20), one has $\alpha\Gamma_0(A_{iI}^* - zI)^{-1}u \in H_+^2(E)$, and since S is an analytic contraction in $\mathbb{C}_+$ the function $S(z)\chi_\varkappa^-\alpha\Gamma_0(A_\varkappa - zI)^{-1}u$, $z \in \mathbb{C}_+$, is an element of $H_+^2(E)$ as long as $\chi_\varkappa^-\alpha\Gamma_0(A_\varkappa - zI)^{-1}u \in H_+^2(E)$. Recalling (34), (36), we conclude that $\chi_\varkappa^+\alpha\Gamma_0(A_\varkappa - zI)^{-1}u \in H_+^2(E)$ and therefore

$$\chi_\varkappa^+\alpha\Gamma_0(A_\varkappa - zI)^{-1}u + \chi_\varkappa^-\alpha\Gamma_0(A_\varkappa - zI)^{-1}u = \alpha\Gamma_0(A_\varkappa - zI)^{-1}u \in H_+^2(E),$$

as required.

The equality

$$\left\{u \in \mathcal{H} : \chi_\varkappa^+\alpha\Gamma_0(A_\varkappa - zI)^{-1}u \in H_-^2(E)\right\} = \left\{u \in \mathcal{H} : \alpha\Gamma_0(A_\varkappa - zI)^{-1}u \in H_-^2(E)\right\}$$

is shown in a similar way. □

The above corollary together with Theorem 5.5 motivates generalising the notion of the absolutely continuous subspace $\mathcal{H}_{\text{ac}}(A_\varkappa)$ to the case of non-selfadjoint extensions $A_\varkappa$ of a symmetric operator A, by identifying it with the set $N_{\text{e}}^\varkappa$. This generalisation follows in the footsteps of the corresponding definition by Naboko [48] in the case of additive perturbations (see also [61, 59] for the general case). In particular, an argument similar to [48, Corollary 1] shows that for the functional model image of $\tilde{N}_{\mathrm{e}}^{\varkappa}$ the following representation holds:

$$\Phi\widetilde{N}_{\mathrm{e}}^{\varkappa} = \Bigg\{ P_K \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} \in \mathfrak{H} : \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} \in \mathfrak{H} \text{ satisfies } \Phi(A_\varkappa - zI)^{-1}\Phi^* P_K \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} = P_K \frac{1}{\cdot - z} \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} \quad \forall z \in \mathbb{C}_- \cup \mathbb{C}_+ \Bigg\}. \tag{37}$$

(Note that the inclusion of the right-hand side of (37) into $\Phi\tilde{N}_{\mathrm{e}}^{\varkappa}$ follows immediately from Theorem 4.2.) Further, we arrive at an equivalent description:

$$\Phi\widetilde{N}_{\mathrm{e}}^{\varkappa} = \left\{ P_K \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} : \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} \in \mathfrak{H} \text{ satisfies } \chi_\varkappa^+(\widetilde{g} + S^* g) + \chi_\varkappa^-(S\widetilde{g} + g) = 0 \right\}. \tag{38}$$

Definition 4. For a symmetric operator A, in the case of a non-selfadjoint extension $A_\varkappa$ the absolutely continuous subspace $\mathcal{H}_{\mathrm{ac}}(A_\varkappa)$ is defined by the formula $\mathcal{H}_{\mathrm{ac}}(A_\varkappa) = N_{\mathrm{e}}^{\varkappa}$.

In the case of a self-adjoint extension $A_\varkappa$, we understand $\mathcal{H}_{\mathrm{ac}}(A_\varkappa)$ in the sense of the classical definition of the absolutely continuous subspace of a self-adjoint operator.

5. The relationship between the set of smooth vectors and the absolutely continuous subspace in the self-adjoint setting

The argument of this section is similar to that of [48], subject to appropriate modifications in order to account for the fact that we deal with extensions of symmetric operators rather than additive perturbations. The same strategy seems to be applicable in the 'mixed' case that incorporates both extensions and perturbations, which has recently been studied in [10].

The following proposition is contained in the proof of [48, Lemma 5]. For the reader's convenience, we provide its proof in Appendix.

Proposition 5.1. *If the Borel transform of a Borel measure μ*

$$\int_{\mathbb{R}} \frac{d\mu(s)}{s - z}$$

is either an element of H_+^2 when $z \in \mathbb{C}_+$ or an element of H_-^2 when $z \in \mathbb{C}_-$, then μ is absolutely continuous with respect to the Lebesgue measure.

Lemma 5.2. *Assume that $\varkappa = \varkappa^*$, $\ker(\alpha) = \{0\}$ and let P_S be the orthogonal projection onto the singular subspace of $A_\varkappa$. Then following inclusion holds:*

$$P_S \widetilde{N}_{\mathrm{e}}^{\varkappa} \subset \bigcap_{z \in \mathbb{C}\setminus\mathbb{R}} \operatorname{ran}(A - zI)\,.$$

Proof. We first demonstrate the validity of the claim for $\varkappa = 0$.

We decompose each smooth vector u (i.e. $u \in \widetilde{N}_{\rm e}^{\varkappa}$) into its projections onto the absolutely continuous and singular subspaces of A_0, that is, $u = u_{\rm ac} + u_s$, where $u_{\rm ac} \in \mathcal{H}_{\rm ac}(A_0)$ and $u_s \in \mathcal{H}_s(A_0)$, so $u_{\rm ac} \perp u_s$ and $u_s \in P_S \widetilde{N}_{\rm e}^{\varkappa}$.

Consider an arbitrary $w \in \mathcal{K}$ and note that, due to the surjectivity of Γ_1, there exists a vector $v \in \operatorname{dom}(A^*)$ such that $\alpha w = \Gamma_1 v$, and therefore

$$
\begin{aligned}
&\left\langle \Gamma_0 (A_0 - zI)^{-1} u, \alpha w \right\rangle_{\mathcal{K}} \\
&\quad = \left\langle \Gamma_0 (A_0 - zI)^{-1} u, \Gamma_1 v \right\rangle_{\mathcal{K}} && (39)\\
&\quad = \left\langle \Gamma_0 (A_0 - zI)^{-1} u, \Gamma_1 v \right\rangle_{\mathcal{K}} - \left\langle \Gamma_1 (A_0 - zI)^{-1} u, \Gamma_0 v \right\rangle_{\mathcal{K}} && (40)\\
&\quad = \left\langle (A_0 - zI)^{-1} u, A^* v \right\rangle_{\mathcal{H}} - \left\langle A^* (A_0 - zI)^{-1} u, v \right\rangle_{\mathcal{H}} && (41)\\
&\quad = \int_{\mathbb{R}} \frac{1}{t-z} d\mu_{u,A^*v}(t) - \int_{\mathbb{R}} \frac{t}{t-z} d\mu_{u,v}(t) = \int_{\mathbb{R}} \frac{1}{t-z} d\hat{\mu}(t). && (42)
\end{aligned}
$$

Here

$$
\mu_{u,A^*v}(\delta) := \langle E_{A_0}(\delta) u, A^* v \rangle_{\mathcal{H}}, \quad \mu_{u,v}(\delta) := \langle E_{A_0}(\delta) u, v \rangle_{\mathcal{H}} \quad \forall \text{ Borel } \delta \subset \mathbb{R},
$$

where E_{A_0} is the spectral resolution of the identity for the operator A_0, and $\hat{\mu}(t) := \mu_{u,A^*v}(t) - t\mu_{u,v}(t)$. Furthermore, the measure $\hat{\mu}$ admits the decomposition into its absolutely continuous and singular parts with respect to the Lebesgue measure. Its singular part is equal to $\mu_{u_s,A^*v}(t) - t\mu_{u_s,v}(t) =: \hat{\mu}_s(t)$, see e.g. [6]. The equality (39)–(40) is due to the observation that Γ_1 vanishes on $\operatorname{dom}(A_0)$, and the equality (40)–(41) is a consequence of the 'Green formula' (3) and the fact that $A \subset A_0$.

At the same time, it follows from Corollary 4.4 that the scalar analytic function $\left\langle \Gamma_0 (A_0 - zI)^{-1} u, \alpha w \right\rangle_{\mathcal{K}}$ is an element of H^2_+ for $z \in \mathbb{C}_+$ and also of H^2_- for $z \in \mathbb{C}_-$. Therefore, by Proposition 5.1 we infer from (39)–(42) that the measure $\hat{\mu}$ is absolutely continuous, which implies that its singular part $\hat{\mu}_s$ is the zero measure.

Finally, we invoke (39)–(42) once again, having replaced u by u_s and $\hat{\mu}$ by $\hat{\mu}_s$, and conclude that

$$
\left\langle \Gamma_0 (A_0 - zI)^{-1} u_s, \alpha w \right\rangle_{\mathcal{K}} = 0 \quad \forall z \in \mathbb{C} \setminus \mathbb{R}. \tag{43}
$$

Now, by virtue of the facts that $w \in \mathcal{K}$ in (43) is arbitrary and $\ker(\alpha) = \{0\}$, it follows that $\Gamma_0 (A_0 - zI)^{-1} u_s = 0$, and since $(A_0 - zI)^{-1} u_s \in \operatorname{dom}(A_0)$ and therefore $\Gamma_1 (A_0 - zI)^{-1} u_s = 0$ automatically, we obtain $(A_0 - zI)^{-1} u_s \in \operatorname{dom}(A)$. Finally, since $A_0 \supset A$, we conclude that $u_s \in \operatorname{ran}(A - zI)$ for all $z \in \mathbb{C} \setminus \mathbb{R}$, as claimed.

In order to treat the case of an arbitrary $\varkappa \in \mathcal{B}(\mathcal{K})$ such that $\varkappa = \varkappa^*$, we define 'shifted' boundary operators $\widehat{\Gamma}_0 := \Gamma_0$, $\widehat{\Gamma}_1 := \Gamma_1 - B_\varkappa \Gamma_0$. Notice that (cf. (4))

$$
\operatorname{dom}(A_\varkappa) = \{u \in \mathcal{H} : \Gamma_1 u = B_\varkappa \Gamma_0 u\} = \{u \in \mathcal{H} : \widehat{\Gamma}_1 u = 0\},
$$

i.e. the operator $A_\varkappa$ plays the rôle of the operator A_0 in the triple $(\mathcal{K}, \widehat{\Gamma}_0, \widehat{\Gamma}_1)$. Further, note that the change of the triple results in a change of the operator that needs to play the rôle of A_{iI}, the dissipative extension used to construct the functional model, which in terms of the 'old' triple $(\mathcal{K}, \Gamma_0, \Gamma_1)$ should be the extension A_B with $B = \alpha(i+\varkappa)\alpha/2$. Repeating the above argument in this new functional model and bearing in mind that the characterisation of $\widetilde{N}_{\mathrm{e}}^{\varkappa}$ in Corollary 4.4 holds for all $\varkappa$, yields the stated result. □

An immediate consequence of this result and the criterion of complete non-selfadjointness (1) is the following assertion.

Corollary 5.3. *Let $\varkappa$ and α be as in the preceding lemma. If A is completely non-selfadjoint, then*

$$\widetilde{N}_{\mathrm{e}}^{\varkappa} \subset \mathcal{H}_{\mathrm{ac}}(A_\varkappa)\,.$$

We now proceed to the proof of the opposite inclusion.

Lemma 5.4 (Modified Rosenblum lemma, cf. [58]**).** *Let β be a self-adjoint operator in a Hilbert space $\mathcal{H}_1$. Suppose that the operator T, defined on* $\mathrm{dom}(\beta)$ *and taking values in a Hilbert space $\mathcal{H}_2$, is such that $T(\beta - z_0 I)^{-1}$ is a Hilbert–Schmidt operator for some $z_0 \in \rho(\beta)$. Then there exists a set $\mathcal{D}$, dense in $\mathcal{H}_{\mathrm{ac}}(\beta)$, such that*

$$\int_{\mathbb{R}} \|T\exp(-i\beta t)u\|^2\, dt < \infty$$

for all $u \in \mathcal{D}$.

Proof. Let $x \in \mathbb{R}$ and $\epsilon > 0$. By Hilbert's first identity,

$$T(\beta - (x+\mathrm{i}\epsilon)I)^{-1} = ((x+\mathrm{i}\epsilon) - z_0)T(\beta - z_0 I)^{-1}(\beta - (x+\mathrm{i}\epsilon)I)^{-1} + T(\beta - z_0 I)^{-1}.$$

Consider the first term on the right-hand side of this last equation. By [49], for every f in $\mathcal{H}_1$ the limit

$$\lim_{\epsilon\to 0} T(\beta - z_0 I)^{-1}(\beta - (x+\mathrm{i}\epsilon)I)^{-1} f$$

exists for almost all $x \in \mathbb{R}$ (the convergence set actually depends on f). It follows that the limit

$$\lim_{\epsilon\to 0} T\left((\beta - (x+\mathrm{i}\epsilon)I)^{-1} - (\beta - (x-\mathrm{i}\epsilon)I)^{-1}\right) f =: F(x)$$

exists for all $f \in \mathcal{H}_1$ and almost all $x \in \mathbb{R}$.

Now, define the set

$$\mathcal{X}(n) := \left\{x \in \mathbb{R} : |x| < n, \|F(x)\| < n\right\}$$

If E_β denotes the spectral measure of the operator β, then the set

$$\mathcal{D} := \bigcup_{n\in\mathbb{N}} E_\beta\big(\mathcal{X}(n)\big)\mathcal{H}_{\mathrm{ac}}(\beta)$$

is dense in $\mathcal{H}_{\rm ac}(\beta)$. Consider an orthonormal basis $\{\phi_k\}$ in $\mathcal{H}_2$ and an arbitrary element $f \in \mathcal{D}$, then, for all k,

$$\begin{aligned}\langle T\exp(-i\beta t)f, \phi_k\rangle &= \int_{\mathcal{X}(n)} e^{-{\rm i}xt}\frac{d}{dx}\langle E_\beta(x)f, T^*\phi_k\rangle\,dx \\ &= \int_{\mathcal{X}(n)} e^{-{\rm i}xt}\langle F(x), T^*\phi_k\rangle\,dx\,,\end{aligned}$$

where in the last equality we have used the fact that by the spectral theorem

$$\lim_{\epsilon\to 0}\left\langle \left((\beta-(x+{\rm i}\epsilon)I)^{-1}-(\beta-(x-{\rm i}\epsilon)I)^{-1}\right)f,\phi\right\rangle = \frac{d}{dx}\langle E_\beta(x)f,\phi\rangle$$

for all $f \in \mathcal{H}_{\rm ac}(\beta)$ and for all $\phi \in \mathcal{H}_1$.

By the Parseval identity one has

$$\int_{\mathbb{R}} |\langle T\exp(-i\beta t)f, \phi_k\rangle|^2\,dt = 2\pi\int_{\mathcal{X}(n)} |\langle F(x), \phi_k\rangle|^2\,dx$$

for all k, which immediately implies that

$$\int_{\mathbb{R}} \|T\exp(-i\beta t)u\|^2\,dt = 2\pi\int_{\mathcal{X}(n)} \|F(x)\|^2\,dx \le 4\pi n^3 < +\infty\,.$$

□

Combining the above statements yields the following result.

Theorem 5.5. *Assume that* $\varkappa = \varkappa^*$, $\ker(\alpha) = \{0\}$ *and let* $\alpha\Gamma_0(A_\varkappa - zI)^{-1}$ *be a Hilbert–Schmidt operator for at least one point* $z \in \rho(A_\varkappa)$. *If* A *is completely non-selfadjoint, then our definition of the absolutely continuous subspace is equivalent to the classical definition of the absolutely continuous subspace of a self-adjoint operator, i.e.*

$$N_{\rm e}^{\varkappa} = \mathcal{H}_{\rm ac}(A_\varkappa)\,.$$

Proof. By applying the Fourier transform to the functions $\mathbb{1}_\pm(t)\alpha\Gamma_0 e^{iA_\varkappa t}e^{\mp\epsilon t}u$, $t \in \mathbb{R}$, where $\mathbb{1}_\pm$ is the characteristic function of $\mathbb{R}_\pm$ and $\epsilon > 0$ is arbitrarily small, one obtains

$$\left\|\alpha\Gamma_0(A_\varkappa - zI)^{-1}u\right\|^2_{H^2_-} + \left\|\alpha\Gamma_0(A_\varkappa - zI)^{-1}u\right\|^2_{H^2_+} = 2\pi\int_{\mathbb{R}}\|\alpha\Gamma_0\exp(iA_\varkappa t)u\|^2\,dt$$

which by Lemma 5.4 is finite for all u in a dense subset of $\mathcal{H}_{\rm ac}(A_\varkappa)$. Hence, in view of Corollary 4.4 and performing closure, one has $\mathcal{H}_{\rm ac}(A_\varkappa) \subset N_{\rm e}^{\varkappa}$. Taking into account Corollary 5.3 completes the proof. □

Remark 5. Alternative conditions, which are less restrictive in general, that guarantee the validity of the assertion of Theorem 5.5 can be obtained along the lines of [50].

6. Wave and scattering operators

The results of the preceding sections allow us to calculate the wave operators for any pair $A_{\varkappa_1}, A_{\varkappa_2}$, where $A_{\varkappa_1}$ and $A_{\varkappa_2}$ are operators in the class introduced in Sect. 2, under the additional assumption that the operator α (see (5)) has a trivial kernel. For simplicity, in what follows we set $\varkappa_2 = 0$ and write $\varkappa$ instead of $\varkappa_1$. Note that A_0 is a self-adjoint operator, which is convenient for presentation purposes.

We begin by establishing the model representation for the function $\exp(iA_\varkappa t)$, $t \in \mathbb{R}$, of the operator $A_\varkappa$, evaluated on the set of smooth vectors $\widetilde{N}_{\rm e}^{\varkappa}$.

Proposition 6.1 ([48, Proposition 2]). *For all $t \in \mathbb{R}$ and $\binom{\widetilde{g}}{g}$ such that $\Phi^* P_K \binom{\widetilde{g}}{g} \in \widetilde{N}_{\rm e}^{\varkappa}$, one has*

$$\Phi \exp(iA_\varkappa t)\Phi^* P_K \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} = P_K \exp(ikt) \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix}.$$

Proof. We use the definition

$$\exp(iA_\varkappa t) := \operatorname*{s-lim}_{n\to+\infty} \left(I - \frac{iA_\varkappa t}{n} \right)^{-n}, \quad t \in \mathbb{R},$$

giving in general an unbounded operator (see [29]). Due to Theorem 4.2, if $\binom{\widetilde{g}}{g} \in \mathfrak{N}_+^{\varkappa} \cap \mathfrak{N}_-^{\varkappa}$, i.e. $\Phi^* P_K \binom{\widetilde{g}}{g} \in \widetilde{N}_{\rm e}^{\varkappa}$, then

$$\left(I - \frac{iA_\varkappa t}{n} \right)^{-n} \Phi^* P_K \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} = \Phi^* P_K \left(1 - \frac{ikt}{n} \right)^{-n} \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix}, \quad t \in \mathbb{R}.$$

Thus, to complete the proof it remains to show that

$$\left\| \left(\exp(ikt) - \left(1 - \frac{ikt}{n} \right)^{-n} \right) \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} \right\|_{\mathfrak{H}} \xrightarrow[n\to\infty]{} 0, \quad t \in \mathbb{R},$$

which follows directly from Lebesgue's dominated convergence theorem. □

Proposition 6.2 ([48, Sect. 4]). *If $\Phi^* P_K \binom{\widetilde{g}}{g} \in \widetilde{N}_{\rm e}^{\varkappa}$ and $\Phi^* P_K \binom{\widehat{g}}{g} \in \widetilde{N}_{\rm e}^{0}$ (with the same element[1] g), then*

$$\left\| \exp(-iA_\varkappa t)\Phi^* P_K \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} - \exp(-iA_0 t)\Phi^* P_K \begin{pmatrix} \widehat{g} \\ g \end{pmatrix} \right\|_{\mathfrak{H}} \xrightarrow[t\to-\infty]{} 0.$$

[1]Despite the fact that $\binom{\widetilde{g}}{g} \in \mathfrak{H}$ is nothing but a symbol, still $\widetilde{g}$ and g can be identified with vectors in certain $L^2(E)$ spaces with operators "weights", see details below in Sect. 7. Further, we recall that even then for $\binom{\widetilde{g}}{g} \in \mathfrak{H}$, the components $\widetilde{g}$ and g are not, in general, *independent* of each other.

Proof. Clearly, $\widetilde{g}-\widehat{g}\in L^2(E)$ since $\binom{\widetilde{g}-\widehat{g}}{0}\in\mathfrak{H}$. Therefore, for all $t\in\mathbb{R}$, we obtain

$$\begin{aligned}
&\left\|\exp(-iA_\varkappa t)\Phi^*P_K\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix}-\exp(-iA_0t)\Phi^*P_K\begin{pmatrix}\widehat{g}\\ g\end{pmatrix}\right\|_{\mathfrak{H}}\\
&\quad=\left\|P_Ke^{-it\cdot}\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix}-P_Ke^{-it\cdot}\begin{pmatrix}\widehat{g}\\ g\end{pmatrix}\right\|_{\mathfrak{H}}\\
&\quad=\left\|P_K\begin{pmatrix}e^{-it\cdot}(\widetilde{g}-\widehat{g})\\ 0\end{pmatrix}\right\|_{\mathfrak{H}}\\
&\quad\le\left\|P_-e^{-it\cdot}(\widetilde{g}-\widehat{g})\right\|_{L^2(E)}\,.
\end{aligned}$$

where in the inequality we use the fact that

$$\left\|P_K\begin{pmatrix}\breve{g}\\ 0\end{pmatrix}\right\|_{\mathfrak{H}}^2=\int_{\mathbb{R}}\left(\left\|P_-\breve{g}(s)\right\|_E^2-\left\|P_-S(s)\breve{g}(s)\right\|_E^2\right)ds\quad\forall\begin{pmatrix}\breve{g}\\ 0\end{pmatrix}\in\mathfrak{H}.$$

Finally, since $\exp(-it\cdot)\in H_+^\infty$ for $t\ge 0$, the convergence (see e.g. [34])

$$\left\|P_-e^{-it\cdot}(\widetilde{g}-\widehat{g})\right\|_{L^2(E)}^2=\int_{-\infty}^t\left\|\mathcal{F}(\widetilde{g}-\widehat{g})(\tau)\right\|_E^2d\tau\xrightarrow[t\to-\infty]{}0$$

holds, where $\mathcal{F}(\widetilde{g}-\widehat{g})$ stands for the Fourier transform of the function $\widetilde{g}-\widehat{g}$. □

It follows from Proposition 6.2 that whenever $\Phi^*P_K\binom{\widetilde{g}}{g}\in\widetilde{N}_{\mathrm{e}}^\varkappa$ and $\Phi^*P_K\binom{\widehat{g}}{g}\in\widetilde{N}_{\mathrm{e}}^0$ (with the same second component g), formally one has

$$\begin{aligned}
\lim_{t\to-\infty}e^{iA_0t}e^{-iA_\varkappa t}\Phi^*P_K\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix}&=\Phi^*P_K\begin{pmatrix}\widehat{g}\\ g\end{pmatrix}\\
&=\Phi^*P_K\begin{pmatrix}-(I+S)^{-1}(I+S^*)g\\ g\end{pmatrix},
\end{aligned}$$

where in the last equality we use the inclusion $\Phi^*P_K\binom{\widehat{g}}{g}\in\widetilde{N}_{\mathrm{e}}^0$, which by (38) yields $\widehat{g}+S^*g+S\widehat{g}+g=0$. In view of the classical definition of the wave operator of a pair of self-adjoint operators, see e.g. [29],

$$W_\pm(A_0,A_\varkappa):=\operatorname*{s-lim}_{t\to\pm\infty}e^{iA_0t}e^{-iA_\varkappa t}P_{\mathrm{ac}}^\varkappa,$$

where $P_{\mathrm{ac}}^\varkappa$ is the projection onto the absolutely continuous subspace of $A^\varkappa$, we obtain that, at least formally, for $\Phi^*P_K\binom{\widetilde{g}}{g}\in\widetilde{N}_{\mathrm{e}}^\varkappa$ one has

$$W_-(A_0,A_\varkappa)\Phi^*P_K\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix}=\Phi^*P_K\begin{pmatrix}-(I+S)^{-1}(I+S^*)g\\ g\end{pmatrix}.\tag{44}$$

By an argument similar to that of Proposition 6.2 (i.e. considering the case $t \to +\infty$), one also obtains

$$\begin{aligned} W_+(A_0, A_\varkappa)\Phi^* P_K \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} &= \lim_{t\to+\infty} e^{iA_0 t} e^{-iA_\varkappa t} \Phi^* P_K \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} \\ &= \Phi^* P_K \begin{pmatrix} \widetilde{g} \\ -(I+S^*)^{-1}(I+S)\widetilde{g} \end{pmatrix} \end{aligned} \tag{45}$$

again for $\Phi^* P_K \binom{\widetilde{g}}{g} \in \widetilde{N}_{\mathrm{e}}^{\varkappa}$.

Further, the definition of the wave operators $W_\pm(A_\varkappa, A_0)$

$$\left\| e^{-iA_\varkappa t} W_\pm(A_\varkappa, A_0)\Phi^* P_K \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} - e^{-iA_0 t}\Phi^* P_K \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} \right\|_{\mathfrak{H}} \xrightarrow[t\to\pm\infty]{} 0$$

yields, for all $\Phi^* P_K \binom{\widetilde{g}}{g} \in \widetilde{N}_{\mathrm{e}}^0$,

$$W_-(A_\varkappa, A_0)\Phi^* P_K \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} = \Phi^* P_K \begin{pmatrix} -(I+\chi_\varkappa^-(S-I))^{-1}(I+\chi_\varkappa^+(S^*-I))g \\ g \end{pmatrix} \tag{46}$$

and

$$W_+(A_\varkappa, A_0)\Phi^* P_K \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} = \Phi^* P_K \begin{pmatrix} \widetilde{g} \\ -(I+\chi_\varkappa^+(S^*-I))^{-1}(I+\chi_\varkappa^-(S-I))\widetilde{g} \end{pmatrix}, \tag{47}$$

where we have used the fact that $\Phi^* P_K \binom{\widetilde{g}}{g} \in \widetilde{N}_{\mathrm{e}}^{\varkappa}$ and the corresponding criterion provided by (38).

In order to rigorously justify the above formal argument, i.e. in order to prove the existence and completeness of the wave operators, one needs to first show that the right-hand sides of the formulae (44)–(47) make sense on dense subsets of the corresponding absolutely continuous subspaces. Noting that (44)–(47) have the form identical to the expressions for wave operators derived in [48, Sect. 4], [50], the remaining part of this justification is a modification of the argument of [50], as follows.

Let $S(z)-I$ be of the class $\mathfrak{S}_\infty(\overline{\mathbb{C}}_+)$, i.e. a compact analytic operator function in the upper half-plane up to the real line. Then so is $(S(z)-I)/2$, which is also uniformly bounded in the upper half-plane along with $S(z)$. We next use the result of [50, Theorem 3] about the non-tangential boundedness of operators of the form $(I+T(z))^{-1}$ for $T(z)$ compact up to the real line. We infer that, provided $(I+(S(z_0)-I)/2)^{-1}$ exists for some $z_0 \in \mathbb{C}_+$ (and hence, see [9], everywhere in $\mathbb{C}_+$ except for a countable set of points accumulating only to the real line), one has non-tangential boundedness of $(I+(S(z)-I)/2)^{-1}$, and therefore also of $(I+S(z))^{-1}$, for almost all points of the real line.

On the other hand, the latter inverse can be computed in $\mathbb{C}_+$:

$$\big(I+S(z)\big)^{-1} = \frac{1}{2}\big(I + i\alpha M(z)^{-1}\alpha/2\big). \tag{48}$$

Indeed, one has

$$\begin{aligned}&\big(I+i\alpha M(z)^{-1}\alpha/2\big)(I+S(z))\\&=2I+i\alpha M(z)^{-1}\alpha+i\alpha\big(B_{iI}^*-M(z)\big)^{-1}\alpha-i\alpha M(z)^{-1}B_{iI}^*\big(B_{iI}^*-M(z)\big)^{-1}\alpha=2I\end{aligned}$$

and the second similar identity for the multiplication in the reverse order proves the claim.

It follows from (48) and the analytic properties of $M(z)$ that the inverse $(I+S(z))^{-1}$ exists everywhere in the upper half-plane. Thus, Theorem 3 of [50] is indeed applicable, which yields that $(I+S(z))^{-1}$ is $\mathbb{R}$-a.e. nontangentially bounded and, by the operator generalisation of the Calderon theorem (see [65]), which was extended to the operator context in [50, Theorem 1], it admits measurable non-tangential limits in the strong operator topology almost everywhere on $\mathbb{R}$. As it is easily seen, these limits must then coincide with $(I+S(k))^{-1}$ for almost all $k\in\mathbb{R}$.

The same argument obviously applies to $(I+S^*(\bar z))^{-1}$ for $z\in\mathbb{C}_-$, where the invertibility follows from the identity

$$\big(I+S^*(\bar z)\big)^{-1}=\frac{1}{2}\big(I-i\alpha M(z)^{-1}\alpha/2\big) \tag{49}$$

obtained exactly as (48), by taking into account analytic properties of $M(z)$.

Finally, the identities

$$(I+\chi_\varkappa^-(S(z)-I))^{-1}=I-i\chi_\varkappa^-\alpha(B_\varkappa-M(z))^{-1}\alpha \tag{50}$$

for $z\in\mathbb{C}_+$ and

$$(I+\chi_\varkappa^+(S^*(\bar z)-I))^{-1}=I+i\chi_\varkappa^+\alpha(B_\varkappa-M(z))^{-1}\alpha \tag{51}$$

for $z\in\mathbb{C}_-$ are used, again by an application of Theorem 3 of [50], to ascertain the existence of bounded $(I+\chi_\varkappa^-(S(k)-I))^{-1}$ and $(I+\chi_\varkappa^+(S^*(k)-I))^{-1}$ almost everywhere on $\mathbb{R}$, provided that the operator $A_\varkappa$ has at least one regular point in each half-plane of the complex plane, see Proposition 2.2. Under the assumptions on S specified above, this latter condition immediately implies that the non-real spectrum of $A_\varkappa$ is countable and accumulates to $\mathbb{R}$ only. (Nevertheless, it could still accumulate to all points of the real line simultaneously.)

The presented argument allows one to verify the correctness of the formulae (44)–(47) for the wave operators. Indeed, for the first of them one considers $\mathbb{1}_n(k)$, the indicator of the set $\{k\in\mathbb{R}:\|(I+S(k))^{-1}\|\le n\}$. Clearly, $\mathbb{1}_n(k)\to 1$ as $n\to\infty$ for almost all $k\in\mathbb{R}$. Next, suppose that $P_K(\tilde g,g)\in\tilde N_{\rm e}^\varkappa$. Then $P_K\mathbb{1}_n(\tilde g,g)$ is also a smooth vector and

$$\begin{pmatrix}-(I+S)^{-1}\mathbb{1}_n(I+S^*)g\\ \mathbb{1}_n g\end{pmatrix}\in\mathfrak{H}.$$

Indeed, for any $(\tilde g, g)\in\mathfrak{H}$ one has

$$\begin{pmatrix}-\mathbb{1}_n(1+S)^{-1}(1+S^*)g\\ \mathbb{1}_n g\end{pmatrix}-\begin{pmatrix}\mathbb{1}_n\tilde g\\ \mathbb{1}_n g\end{pmatrix}$$
$$=\begin{pmatrix}-\mathbb{1}_n(1+S)^{-1}[(\tilde g+S^*g)+(S\tilde g+g)]\\ 0\end{pmatrix}\in\begin{pmatrix}L^2(E)\\ 0\end{pmatrix}\in\mathfrak{H},$$

whereas the inclusion in the set of smooth vectors follows directly from (38). It follows, by the Lebesgue dominated convergence theorem, that the set of vectors $P_K\mathbb{1}_n(\tilde g, g)$ is dense in $N_{\mathrm e}^{\varkappa}$. The remaining three wave operators are treated in a similar way. Finally, the density of the range of the four wave operators follows from the density of their domains, by a standard inversion argument, see e.g. [73].

We have thus proved the following theorem.

Theorem 6.3. *Let A be a closed, symmetric, completely non-selfadjoint operator with equal deficiency indices and consider its extension $A_\varkappa$, as described in Sect.* 2, *under the assumptions that* $\ker(\alpha)=\{0\}$ (*see* (5)) *and that $A_\varkappa$ has at least one regular point in $\mathbb{C}_+$ and in $\mathbb{C}_-$. If $S-I\in\mathfrak{S}_\infty(\overline{\mathbb{C}}_+)$, then the wave operators $W_\pm(A_0,A_\varkappa)$ and $W_\pm(A_\varkappa,A_0)$ exist on dense sets in $N_{\mathrm e}^{\varkappa}$ and $\mathcal{H}_{\mathrm{ac}}(A_0)$, respectively, and are given by the formulae* (44)–(47)*. The ranges of $W_\pm(A_0,A_\varkappa)$ and $W_\pm(A_\varkappa,A_0)$ are dense in $\mathcal{H}_{\mathrm{ac}}(A_0)$ and $N_{\mathrm e}^{\varkappa}$, respectively.*[2]

Remark 6. 1. The identities (48)–(49) can be used to replace the condition $S(z)-I\in\mathfrak{S}_\infty(\overline{\mathbb{C}}_+)$ by the following equivalent condition: $\alpha M(z)^{-1}\alpha$ is nontangentially bounded almost everywhere on the real line, and $\alpha M(z)^{-1}\alpha\in\mathfrak{S}_\infty(\overline{\mathbb{C}}_+)$ for $\Im z\geq 0$. In order to do so, one notes that $(I+T)^{-1}-I=-(I+T)^{-1}T\in\mathfrak{S}_\infty(\overline{\mathbb{C}}_+)$ as long as $T\in\mathfrak{S}_\infty(\overline{\mathbb{C}}_+)$ and $(I+T)^{-1}$ is bounded.

2. The latter condition is satisfied [24], if the scalar function $\|\alpha M(z)^{-1}\alpha\|_{\mathfrak{S}_p}$ is nontangentially bounded almost everywhere on the real line for some $p<\infty$, where $\mathfrak{S}_p$, $p\in(0,\infty]$, are the standard Schatten–von Neumann classes of compact operators.

3. An alternative sufficient condition is the condition $\alpha\in\mathfrak{S}_2$ (and therefore $B_\varkappa\in\mathfrak{S}_1$), or, more generally, $\alpha M(z)^{-1}\alpha\in\mathfrak{S}_1$, see [49] for details.

4. Following from the analysis above, the existence and completeness of the wave operators for the par $A_\varkappa$, A_0 is closely linked to the condition of α having a 'relative Hilbert–Schmidt property' with respect to $M(z)$. Recalling that $B_\varkappa=\alpha\varkappa\alpha/2$, this is not always feasible to expect. Nevertheless, by appropriately modifying the boundary triple, the situation can often be rectified. For example, if $C_\varkappa=C_0+\alpha\varkappa\alpha/2$, where C_0 and $\varkappa$ are bounded and $\alpha\in\mathfrak{S}_2$, replaces the operator $B_\varkappa$ in (5), then one 'shifts' the boundary triple (cf. the proof of Lemma 5.2):

---

[2] In the case when $A_\varkappa$ is self-adjoint, or, in general, the named wave operators are bounded, the claims of the theorem are equivalent (by the classical Banach–Steinhaus theorem) to the statement of the existence and completeness of the wave operators for the pair $A_0, A_\varkappa$. Sufficient conditions of boundedness of these wave operators are contained in e.g. [48, Sect. 4], [50] and references therein.

$\widehat{\Gamma}_0 = \Gamma_0$, $\widehat{\Gamma}_1 = \Gamma_1 - C_0\Gamma_0$. One thus obtains that in the new triple $(\mathcal{K}, \widehat{\Gamma}_0, \widehat{\Gamma}_1)$ the operator $A_\varkappa$ coincides with the extension corresponding to the boundary operator $B_\varkappa = \alpha\varkappa\alpha/2$, whereas the Weyl–Titchmarsh function $M(z)$ undergoes a shift to the function $M(z) - C_0$. The proof of Theorem 6.1 remains intact, while Part 3 of this remark yields that the condition $\alpha(M(z) - C_0)^{-1}\alpha \in \mathfrak{S}_1$ guarantees the existence and completeness of the wave operators for the pair A_{C_0}, $A_{C_\varkappa}$. The fact that the operator A_0 here is replaced by the operator A_{C_0} reflects the standard argument that the complete scattering theory for a pair of operators requires that the operators forming this pair are 'close enough' to each other.

Finally, the scattering operator Σ for the pair $A_\varkappa$, A_0 is defined by

$$\Sigma = W_+^{-1}(A_\varkappa, A_0)W_-(A_\varkappa, A_0).$$

The above formulae for the wave operators lead (cf. [48]) to the following formula for the action of Σ in the model representation:

$$\Phi\Sigma\Phi^* P_K \begin{pmatrix} \tilde{g} \\ g \end{pmatrix} = P_K \begin{pmatrix} -(I + \chi_\varkappa^-(S - I))^{-1}(I + \chi_\varkappa^+(S^* - I))g \\ (I + S^*)^{-1}(I + S)(I + \chi_\varkappa^-(S - I))^{-1}(I + \chi_\varkappa^+(S^* - I))g \end{pmatrix}, \tag{52}$$

whenever $\Phi^* P_K \binom{\tilde{g}}{g} \in \widetilde{N}_\mathrm{e}^0$. In fact, as explained above, this representation holds on a dense linear set in $\widetilde{N}_\mathrm{e}^0$ within the conditions of Theorem 6.3, which guarantees that all the objects on the right-hand side of the formula (52) are correctly defined.

7. Spectral representation for the absolutely continuous part of the operator A_0

The identity

$$\left\| P_K \begin{pmatrix} \tilde{g} \\ g \end{pmatrix} \right\|_{\mathfrak{H}}^2 = \langle (I - S^*S)\tilde{g}, \tilde{g} \rangle$$

which is derived in the same way as in [48, Sect. 7] for all $P_K\binom{\tilde{g}}{g} \in \widetilde{N}_\mathrm{e}^0$ and is equivalent to the condition $(\tilde{g} + S^*g) + (S\tilde{g} + g) = 0$, see (38), allows us to consider the isometry $F : \Phi\widetilde{N}_\mathrm{e}^0 \mapsto L^2(E; I - S^*S)$ defined by the formula

$$FP_K \begin{pmatrix} \tilde{g} \\ g \end{pmatrix} = \tilde{g}. \tag{53}$$

Here $L^2(E; I - S^*S)$ is the Hilbert space of E-valued functions on $\mathbb{R}$ square summable with the matrix 'weight' $I - S^*S$, cf. (22). Similarly, the formula

$$F_* P_K \begin{pmatrix} \tilde{g} \\ g \end{pmatrix} = g$$

defines an isometry F_* from $\Phi\widetilde{N}_\mathrm{e}^0$ to $L^2(E; I - SS^*)$.

Lemma 7.1. *Suppose that the assumptions of Theorem* 6.3 *hold. Then the ranges of the operators F and F_* are dense in the spaces $L^2(E; I - S^*S)$ and $L^2(E; I - SS^*)$, respectively.*

Proof. Indeed, for all $\tilde{g} \in L^2(E; I - S^*S)$ and $g = -S\tilde{g}$ one has $(\tilde{g}, g) \in \mathcal{H}$ with $\|(\tilde{g}, g)\|_{\mathcal{H}} = \|\tilde{g}\|_{L^2(E;I-S^*S)}$. By repeating the proof of Theorem 6.3, the operator $I + S^*$ is boundedly invertible almost everywhere on $\mathbb{R}$.

Now, consider $\mathbb{1}_n(k)$, the indicator of the set $\{k \in \mathbb{R} : \|(I + S^*(k))^{-1}\| \leq n\}$. For $\tilde{g} \in L^2(E; I - S^*S)$ and, as above, $g = -S\tilde{g}$, one has $\mathbb{1}_n(\tilde{g}, -(I + S^*)^{-1}(I + S)\tilde{g}) \in \mathcal{H}$, since

$$\begin{aligned}&\mathbb{1}_n\begin{pmatrix}\tilde{g}\\ -(I+S^*)^{-1}(I+S)\tilde{g}\end{pmatrix} - \mathbb{1}_n\begin{pmatrix}\tilde{g}\\ g\end{pmatrix}\\ &\quad = \begin{pmatrix}0\\ -\mathbb{1}_n(I+S^*)^{-1}\big[(S\tilde{g}+g)+(\tilde{g}+S^*g)\big]\end{pmatrix} \in \begin{pmatrix}0\\ L^2(E)\end{pmatrix}.\end{aligned}$$

Finally, the set $\{\mathbb{1}_n\tilde{g}\}$ is dense in $L^2(E; I - S^*S)$ by the Lebesgue dominated convergence theorem, whereas $P_K\mathbb{1}_n(\tilde{g}, -(I + S^*)^{-1}(I + S)\tilde{g}) \in \widetilde{N}_{\rm e}^0$ by direct calculation. □

Corollary 7.2. *The operator F, respectively F_*, admits an extension to the unitary mapping between $\Phi N_{\rm e}^0$ and $L^2(E; I - S^*S)$, respectively $L^2(E; I - SS^*)$.*

It follows that the operator $(A_0 - z)^{-1}$ (see notation (6)) considered on $\widetilde{N}_{\rm e}^0$ acts as the multiplication by $(k - z)^{-1}$, $k \in \mathbb{R}$, both in $L^2(E; I - S^*S)$ and $L^2(E; I - SS^*)$. In particular, if one considers the absolutely continuous 'part' of the operator A_0, namely the operator $A_0^{(\rm e)} := A_0|_{N_{\rm e}^0}$, then $F\Phi A_0^{(\rm e)}\Phi^*F^*$ and $F_*\Phi A_0^{(\rm e)}\Phi^*F_*^*$ are the operators of multiplication by the independent variable in the spaces $L^2(E; I - S^*S)$ and $L^2(E; I - SS^*)$, respectively.

In order to obtain a spectral representation from the above result, it is necessary to diagonalise the weights in the definitions of the above L^2-spaces. The corresponding transformation is straightforward when $\alpha = \sqrt{2}I$. (This choice of α satisfies the conditions of Theorem 6.3 e.g. when the boundary space $\mathcal{K}$ is finite-dimensional. The corresponding diagonalisation in the general setting of non-negative, bounded α will be treated elsewhere.) In this particular case one has

$$S = (M - iI)(M + iI)^{-1}, \tag{54}$$

and consequently

$$I - S^*S = -2i(M^* - iI)^{-1}(M - M^*)(M + iI)^{-1} \tag{55}$$

and

$$I - SS^* = 2i(M + iI)^{-1}(M^* - M)(M^* - iI)^{-1}.$$

Introducing the unitary transformations

$$G : L^2(E; I - S^*S) \mapsto L^2(E; -2i(M - M^*)), \tag{56}$$

$$G_* : L^2(E; I - SS^*) \mapsto L^2(E; -2i(M - M^*)) \tag{57}$$

by the formulae $g \mapsto (M + iI)^{-1}g$ and $g \mapsto (M^* - iI)^{-1}g$, respectively, one arrives at the fact that $GF\Phi A_0^{(\rm e)}\Phi^*F^*G^*$ and $G_*F_*\Phi A_0^{(\rm e)}\Phi^*F_*^*G_*^*$ are the operators of multiplication by the independent variable in the space $L^2(E; -2i(M - M^*))$.

Remark 7. The weight $M^* - M$ can be assumed to be naturally diagonal in the setting of quantum graphs, see [14] (cf. [18, 19]), including the situation of an infinite number of semi-infinite edges.

The above result only pertains to the absolutely continuous part of the self-adjoint operator A_0, unlike e.g. the passage to the classical von Neumann direct integral, under which the whole of the self-adjoint operator gets mapped to the multiplication operator in a weighted L^2-space (see e.g. [6, Chap. 7]). Nevertheless, it proves useful in scattering theory, since it yields an explicit expression for the scattering matrix $\widehat{\Sigma}$ for the pair $A_\varkappa$, A_0, which is the image of the scattering operator Σ in the spectral representation of the operator A_0. Namely, we prove the following statement.

Theorem 7.3. *The following formula holds:*

$$\widehat{\Sigma} = GF\Sigma(GF)^* = (M-\varkappa)^{-1}(M^*-\varkappa)(M^*)^{-1}M, \tag{58}$$

where the right-hand side represents the operator of multiplication by the corresponding function in the space $L^2(E; -2i(M-M^*))$.

Proof. Using the definition (53) of the isometry F along with the relationship (38) between $\widetilde{g}$ and g whenever $P_K\binom{\widetilde{g}}{g} \in \Phi\widetilde{N}_{\mathrm{e}}^{\varkappa}$ with $\varkappa = 0$, we obtain from (52)

$$F\Sigma F^* = \big(I + \chi_\varkappa^-(S-I)\big)^{-1}\big(I+\chi_\varkappa^+(S^*-I)\big)(I+S^*)^{-1}(I+S), \tag{59}$$

where the right-hand side represents the operator of multiplication by the corresponding function.

Furthermore, substituting the expression (7) for S in terms of M implies that $F\Sigma F^*$ is the operator of multiplication by

$$(M+iI)(M-\varkappa)^{-1}(M^*-\varkappa)(M^*)^{-1}M(M+iI)$$

in the space $L^2(\mathcal{K}; I - S^*S)$. Using (55), we now obtain the following identity for all $f, g \in L^2(\mathcal{K}; I-S^*S)$:

$$\begin{aligned}
&\langle F\Sigma F^* f, g\rangle_{L^2(\mathcal{K};I-S^*S)}\\
&\quad= \big\langle (I-S^*S)(M+iI)(M-\varkappa)^{-1}(M^*-\varkappa)(M^*)^{-1}M(M+iI)f, g\big\rangle\\
&\quad= \big\langle -2i(M^*-iI)^{-1}(M-M^*)(M+iI)^{-1}(M+iI)\\
&\qquad\quad \cdot (M-\varkappa)^{-1}(M^*-\varkappa)(M^*)^{-1}M(M+iI)f, g\big\rangle\\
&\quad= \big\langle -2i(M-M^*)(M-\varkappa)^{-1}(M^*-\varkappa)(M^*)^{-1}M(M+iI)f, (M+iI)g\big\rangle,
\end{aligned}$$

which is equivalent to (58), in view of the definition of the operator G. □

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Appendix

Proof of Theorem 4.1**.** We prove Theorem 4.1(i). The proof of Theorem 4.1(ii) is carried out along the same lines.

For any (v_-, u, v_+) in the space $\mathcal{H}$ given in (26), consider the mappings $\mathcal{F}_\pm : \mathcal{H} \to L^2(\mathbb{R}, E)$ introduced in [60, Sect. 2.1] following the corresponding definitions in [48] and given by

$$\mathcal{F}_+(v_-, u, v_+) = -\frac{1}{\sqrt{2\pi}} \lim_{\epsilon \searrow 0} \alpha \Gamma_0 (A_{\mathrm{i}I} - (\cdot - \mathrm{i}\epsilon)I)^{-1} u + S^* \hat{v}_- + \hat{v}_+ \tag{60}$$

$$\mathcal{F}_-(v_-, u, v_+) = -\frac{1}{\sqrt{2\pi}} \lim_{\epsilon \searrow 0} \alpha \Gamma_0 (A_{\mathrm{i}I}^* - (\cdot + \mathrm{i}\epsilon)I)^{-1} u + \hat{v}_- + S\hat{v}_+ \,, \tag{61}$$

where $\hat{v}_\pm$ are the Fourier transforms of $v_\pm \in L^2(\mathbb{R}_\pm, E)$ extended by zero to $L^2(\mathbb{R}, E)$. Note that the limits exist almost everywhere due to (20).

According to [60, Theorem 2.3], if $\binom{\widetilde{g}}{g} = \Phi h$, then

$$\mathcal{F}_+ h = \widetilde{g} + S^* g \,, \quad \mathcal{F}_- h = S\widetilde{g} + g \,. \tag{62}$$

Therefore, for proving Theorem 4.1(i), one should establish the validity of the identities:

$$\mathcal{F}_\pm (A_\varkappa - zI)^{-1} \Phi^{-1} \begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} = \mathcal{F}_\pm \Phi^{-1} P_K \frac{1}{\cdot - z} \begin{pmatrix} \widetilde{g} \\ g - \chi_\varkappa^+ \Theta_\varkappa^{-1}(z)(\widetilde{g} + S^* g)(z) \end{pmatrix} \tag{63}$$

for $z \in \mathbb{C}_- \cap \rho(A_\varkappa)$. First we compute the left-hand-side of (63). It follows from Lemma 3.1(i)–(ii) that, for $z, \lambda \in \mathbb{C}_- \cap \rho(A_\varkappa)$ and $h \in \mathcal{H}$,

$$\begin{aligned}
&\alpha \Gamma_0 (A_{\mathrm{i}I} - zI)^{-1} (A_\varkappa - \lambda I)^{-1} h \\
&\quad = \Theta_\varkappa(z) \alpha \Gamma_0 (A_\varkappa - zI)^{-1} (A_\varkappa - \lambda I)^{-1} h \\
&\quad = \frac{1}{z - \lambda} \Theta_\varkappa(z) \alpha \Gamma_0 \left[(A_\varkappa - zI)^{-1} - (A_\varkappa - \lambda I)^{-1} \right] h \\
&\quad = \frac{1}{z - \lambda} \left[\alpha \Gamma_0 (A_{\mathrm{i}I} - zI)^{-1} - \Theta_\varkappa(z) \alpha \Gamma_0 (A_\varkappa - \lambda I)^{-1} \right] h \\
&\quad = \frac{1}{z - \lambda} \left[\alpha \Gamma_0 (A_{\mathrm{i}I} - zI)^{-1} - \Theta_\varkappa(z) \Theta_\varkappa^{-1}(\lambda) \alpha \Gamma_0 (A_{\mathrm{i}I} - \lambda I)^{-1} \right] h \,.
\end{aligned}$$

Let $z=k-\mathrm{i}\epsilon$ with $k\in\mathbb{R}$, then it follows from the computation above that

$$\begin{aligned}&\lim_{\epsilon\searrow 0}\alpha\Gamma_0(A_{\mathrm{i}I}-(k-\mathrm{i}\epsilon)I)^{-1}(A_\varkappa-\lambda I)^{-1}h\\&=\lim_{\epsilon\searrow 0}\frac{\left[\alpha\Gamma_0(A_{\mathrm{i}I}-(k-\mathrm{i}\epsilon)I)^{-1}-\Theta_\varkappa(k-\mathrm{i}\epsilon)\Theta_\varkappa^{-1}(\lambda)\alpha\Gamma_0(A_{\mathrm{i}I}-\lambda I)^{-1}\right]h}{(k-\mathrm{i}\epsilon)-\lambda}.\end{aligned}$$

Substituting (60) into the last equality, one has

$$\mathcal{F}_+(A_\varkappa-\lambda I)^{-1}h=\frac{1}{\cdot-\lambda}\left[\mathcal{F}_+h-\Theta_\varkappa(\cdot)\Theta_\varkappa^{-1}(\lambda)\mathcal{F}_+h(\lambda)\right].$$

Hence, in view of (62), one concludes

$$\mathcal{F}_+(A_\varkappa-\lambda I)^{-1}\Phi^{-1}\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix}=\frac{1}{\cdot-\lambda}\left[\widetilde{g}+S^*g-\Theta_\varkappa(\cdot)\Theta_\varkappa^{-1}(\lambda)(\widetilde{g}+S^*g)(\lambda)\right]. \tag{64}$$

On the basis of Lemma 3.1(iii)–(iv) and reasoning in the same fashion as was done to obtain (64), one verifies

$$\mathcal{F}_-(A_\varkappa-\lambda I)^{-1}\Phi^{-1}\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix}=\frac{1}{\cdot-\lambda}\left[S\widetilde{g}+g-\widehat{\Theta}_\varkappa(\cdot)\Theta_\varkappa^{-1}(\lambda)(\widetilde{g}+S^*g)(\lambda)\right]. \tag{65}$$

Let us focus on the right hand side of (63). Note that

$$\begin{aligned}&P_K\frac{1}{\cdot-z}\begin{pmatrix}\widetilde{g}\\ g-\chi_\varkappa^+\Theta_\varkappa^{-1}(z)(\widetilde{g}+S^*g)(z)\end{pmatrix}\\&=\begin{pmatrix}\frac{\widetilde{g}}{\cdot-z}-P_+\frac{1}{\cdot-z}[\widetilde{g}+S^*g-S^*\chi_\varkappa^+\Theta_\varkappa^{-1}(z)(\widetilde{g}+S^*g)(z)]\\ \frac{1}{\cdot-z}(g-\chi_\varkappa^+\Theta_\varkappa^{-1}(z)(\widetilde{g}+S^*g)(z))-P_-\frac{1}{\cdot-z}[S\widetilde{g}+g-\chi_\varkappa^+\Theta_\varkappa^{-1}(z)(\widetilde{g}+S^*g)(z)]\end{pmatrix}\\&=\frac{1}{\cdot-z}\begin{pmatrix}\widetilde{g}-(\widetilde{g}+S^*g)(z)+S^*(\overline{z})\chi_\varkappa^+\Theta_\varkappa^{-1}(z)(\widetilde{g}+S^*g)(z)\\ g-\chi_\varkappa^+\Theta_\varkappa^{-1}(z)(\widetilde{g}+S^*g)(z)\end{pmatrix}\end{aligned} \tag{66}$$

where (25) is used in the first equality and in the second the fact that if f is a function in H^2_-, then, for any $z\in\mathbb{C}_-$,

$$P_+\left(\frac{f}{\cdot-z}\right)=P_+\left(\frac{f+f(z)-f(z)}{\cdot-z}\right)=P_+\left(\frac{f(z)}{\cdot-z}\right)=\frac{f(z)}{\cdot-z}. \tag{67}$$

Now, apply $\mathcal{F}_+\Phi^{-1}$ to (66) taking into account (62):

$$\begin{aligned}&\mathcal{F}_+\Phi^{-1}\frac{1}{\cdot-z}\begin{pmatrix}\widetilde{g}-(\widetilde{g}+S^*g)(z)+S^*(\overline{z})\chi_\varkappa^+\Theta_\varkappa^{-1}(z)(\widetilde{g}+S^*g)(z)\\ g-\chi_\varkappa^+\Theta_\varkappa^{-1}(z)(\widetilde{g}+S^*g)(z)\end{pmatrix}\\&\quad=\frac{1}{\cdot-z}[\widetilde{g}+S^*g-(\widetilde{g}+S^*g)(z)+(S^*(\overline{z})-S^*)\chi_\varkappa^+\Theta_\varkappa^{-1}(z)(\widetilde{g}+S^*g)(z)]\\&\quad=\frac{1}{\cdot-z}[\widetilde{g}+S^*g-(\Theta_\varkappa(z)-(S^*(\overline{z})-S^*)\chi_\varkappa^+)\Theta_\varkappa^{-1}(z)(\widetilde{g}+S^*g)(z)]\\&\quad=\frac{1}{\cdot-z}[\widetilde{g}+S^*g-\Theta(\cdot)\Theta_\varkappa^{-1}(z)(\widetilde{g}+S^*g)(z)].\end{aligned}$$

By combining the last equality with (64), we have established the first identity in (63).

Now, if one applies $\mathcal{F}_-\Phi^{-1}$ to (66), then, in view of (62), one has

$$\mathcal{F}_-\Phi^{-1}\frac{1}{\cdot - z}\begin{pmatrix}\widetilde{g} - (\widetilde{g}+S^*g)(z) + S^*(\overline{z})\chi_\varkappa^+\Theta_\varkappa^{-1}(z)(\widetilde{g}+S^*g)(z)\\ g - \chi_\varkappa^+\Theta_\varkappa^{-1}(z)(\widetilde{g}+S^*g)(z)\end{pmatrix}$$
$$= \frac{1}{\cdot - z}[S\widetilde{g} + g - S(\widetilde{g}+S^*g)(z) - (I - SS^*(\overline{z}))\chi_\varkappa^+\Theta_\varkappa^{-1}(z)(\widetilde{g}+S^*g)(z)]$$
$$= \frac{1}{\cdot - z}[S\widetilde{g} + g - (S\Theta_\varkappa(z) + \chi_\varkappa^+ - SS^*(\overline{z})\chi_\varkappa^+)\Theta_\varkappa^{-1}(z)(\widetilde{g}+S^*g)(z)]$$
$$= \frac{1}{\cdot - z}[S\widetilde{g} + g - (S\chi_\varkappa^- + \chi_\varkappa^-)\Theta_\varkappa^{-1}(z)(\widetilde{g}+S^*g)(z)]$$
$$= \frac{1}{\cdot - z}[S\widetilde{g} + g - \widehat{\Theta}_\varkappa(\cdot)\Theta_\varkappa^{-1}(z)(\widetilde{g}+S^*g)(z)]$$

Thus, after comparing this last equality with (65), we arrive at the second identity in (63).

Proof of Theorem 4.2**.** Let us first show that the following inclusion holds

$$\mathfrak{N}_\pm^\varkappa \subset \left\{\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} \in \mathfrak{H} : \Phi(A_\varkappa - zI)^{-1}\Phi^* P_K\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} = P_K\frac{1}{\cdot - z}\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} \text{ for all } z \in \mathbb{C}_\pm\right\}$$

Consider $z \in \mathbb{C}_- \cap \rho(A_\varkappa)$. By (25) and Theorem 4.1, one has

$$\Phi(A_\varkappa - zI)^{-1}\Phi^{-1}P_K\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} = \Phi(A_\varkappa - zI)^{-1}\Phi^{-1}\begin{pmatrix}\widetilde{g} - P_+(\widetilde{g}+S^*g)\\ g - P_-(S\,\widetilde{g}+g)\end{pmatrix}$$
$$= P_K\frac{1}{\cdot - z}$$
$$\cdot\begin{pmatrix}\widetilde{g} - P_+(\widetilde{g}+S^*g)\\ g - P_-(S\widetilde{g}+g) - \chi_\varkappa^+\Theta_\varkappa^{-1}(z)\left[\widetilde{g} - P_+(\widetilde{g}+S^*g) + S^*(g - P_-(S\widetilde{g}+g))\right](z)\end{pmatrix}$$

where

$$\left[\widetilde{g} - P_+(\widetilde{g}+S^*g) + S^*(g - P_-(S\widetilde{g}+g))\right](z)$$

is to be understood as the analytic continuation into the lower half-plane of the function

$$\widetilde{g} - P_+(\widetilde{g}+S^*g) + S^*(g - P_-(S\widetilde{g}+g)) = P_-(\widetilde{g}+S^*g) - S^*P_-(S\widetilde{g}+g), \quad (68)$$

which is clearly an element of $H^2_-(E)$. Thus,

$$\Phi(A_\varkappa - zI)^{-1}\Phi^{-1}P_K\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} = P_K\frac{1}{\cdot - z}\begin{pmatrix}\widetilde{g} - P_+(\widetilde{g}+S^*g)\\ g - P_-(S\widetilde{g}+g) - \gamma(z)\end{pmatrix} \quad (69)$$

where

$$\gamma(z) := \chi_\varkappa^+\Theta_\varkappa^{-1}(z)\big(P_-(\widetilde{g}+S^*g)(z) - S^*P_-(S\widetilde{g}+g)(z)\big). \quad (70)$$

The following lemma is needed to simplify the form of $\gamma(z)$.

Lemma A.1. *For all* $\binom{\widetilde{g}}{g} \in \mathfrak{H}$ *the following identity holds:*

$$\gamma(z) = -P_-(S\widetilde{g} + g)(z) \quad \forall z \in \mathbb{C}_-.$$

Proof.

$$\begin{aligned}
&\chi_\varkappa^+ \Theta_\varkappa^{-1}(z)\bigl(P_-(\widetilde{g} + S^* g)(z) - S^*(\overline{z})P_-(S\widetilde{g} + g)(z)\bigr) \\
&= \chi_\varkappa^+\bigl(I + i\alpha(B_\varkappa - M(z))^{-1}\alpha\chi_\varkappa^+\bigr)\bigl(P_-(\widetilde{g} + S^* g)(z) - S^*(\overline{z})P_-(S\widetilde{g} + g)(z)\bigr) \\
&= \bigl(I + i\chi_\varkappa^+\alpha(B_\varkappa - M(z))^{-1}\alpha\bigr)\chi_\varkappa^+\bigl(P_-(\widetilde{g} + S^* g)(z) - S^*(\overline{z})P_-(S\widetilde{g} + g)(z)\bigr) \\
&= \bigl(I + \chi_\varkappa^+(S^*(\overline{z}) - I)\bigr)^{-1}\bigl(\chi_\varkappa^+ P_-(\widetilde{g} + S^* g)(z) - \chi_\varkappa^+ S^*(\overline{z})P_-(S\widetilde{g} + g)(z)\bigr) \\
&= \bigl(I + \chi_\varkappa^+(S^*(\overline{z}) - I)\bigr)^{-1}\bigl(-\chi_\varkappa^- P_-(S\widetilde{g} + g)(z) - \chi_\varkappa^+ S^*(\overline{z})P_-(S\widetilde{g} + g)(z)\bigr) \\
&= \bigl(I + \chi_\varkappa^+(S^*(\overline{z}) - I)\bigr)^{-1}\bigl(-\chi_\varkappa^- - \chi_\varkappa^+ S^*(\overline{z})\bigr)P_-(S\widetilde{g} + g)(z) \\
&= -P_-(S\widetilde{g} + g)(z),
\end{aligned}$$

where we use the fact that

$$I + i\chi_\varkappa^+\alpha(B_\varkappa - M(z))^{-1}\alpha = \bigl(I + \chi_\varkappa^+(S^*(\overline{z}) - I)\bigr)^{-1},$$

proved in a similar way to (16). □

Therefore, for $\binom{\widetilde{g}}{g} \in \mathfrak{N}_-^\varkappa$ the expression (69) can be rewritten as

$$\begin{aligned}
\Phi(A_\varkappa - zI)^{-1}\Phi^{-1}P_K\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} &= P_K\frac{1}{\cdot - z}\begin{pmatrix}\widetilde{g} - P_+(\widetilde{g} + S^* g)\\ g - P_-(S\widetilde{g} + g) + P_-(S\widetilde{g} + g)(z)\end{pmatrix} \\
&= P_K\frac{1}{\cdot - z}\left[\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} - \begin{pmatrix}P_+(\widetilde{g} + S^* g)\\ P_-(S\widetilde{g} + g) - P_-(S\widetilde{g} + g)(z)\end{pmatrix}\right].
\end{aligned}$$

One completes the proof by observing that

$$\frac{P_+(\widetilde{g} + S^* g)}{\cdot - z} \in H_+^2(E), \qquad \frac{P_-(S\widetilde{g} + g) - P_-(S\widetilde{g} + g)(z)}{\cdot - z} \in H_-^2(E).$$

We have thus shown that

$$\mathfrak{N}_-^\varkappa \subset \left\{\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} \in \mathfrak{H} : \Phi(A_\varkappa - zI)^{-1}\Phi^* P_K\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} = P_K\frac{1}{\cdot - z}\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} \text{ for all } z \in \mathbb{C}_-\right\}.$$

The inclusion

$$\mathfrak{N}_+^\varkappa \subset \left\{\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} \in \mathfrak{H} : \Phi(A_\varkappa - zI)^{-1}\Phi^* P_K\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} = P_K\frac{1}{\cdot - z}\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} \text{ for all } z \in \mathbb{C}_+\right\}$$

is proved analogously.

To prove the converse inclusion, i.e.

$$\left\{\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} \in \mathfrak{H} : \Phi(A_\varkappa - zI)^{-1}\Phi^* P_K\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} = P_K\frac{1}{\cdot - z}\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} \text{ for all } z \in \mathbb{C}_\pm\right\} \subset \mathfrak{N}_\pm^\varkappa$$

one again follows the arguments of [48, Theorem 4]. According to (69), for all $z \in \mathbb{C}_- \cap \rho(A_\varkappa)$, one has

$$\Phi(A_\varkappa - zI)^{-1}\Phi^{-1}P_K\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} = P_K\frac{1}{\cdot - z}\begin{pmatrix}\widetilde{g} - P_+(\widetilde{g} + S^*g)\\ g - P_-(S\widetilde{g} + g) - \gamma(z)\end{pmatrix},$$

where $\gamma(z)$ is defined in (70). Denoting $\widehat{\gamma} := \gamma + P_-(S\widetilde{g} + g)$, it follows from (25) that

$$\Phi(A_\varkappa - zI)^{-1}\Phi^{-1}P_K\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} - P_K\frac{1}{\cdot - z}\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} = P_K\begin{pmatrix}0\\ -\widehat{\gamma}(z)(\cdot - z)^{-1}\end{pmatrix}$$
$$= \begin{pmatrix}P_+(S^*\widehat{\gamma}(z)(\cdot - z)^{-1})\\ -\widehat{\gamma}(z)(\cdot - z)^{-1} + P_-(\widehat{\gamma}(z)(\cdot - z)^{-1})\end{pmatrix}.$$

Furthermore, in view of (67), one has

$$P_+\left[\frac{S^*\widehat{\gamma}(z)}{\cdot - z}\right] = \frac{S^*(\overline{z})\widehat{\gamma}(z)}{\cdot - z}$$

and, clearly,

$$P_-\left[\frac{\widehat{\gamma}(z)}{\cdot - z}\right] = 0\,.$$

Therefore

$$\Phi(A_\varkappa - zI)^{-1}\Phi^{-1}P_K\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} - P_K\frac{1}{\cdot - z}\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} = \begin{pmatrix}S^*(\overline{z})\widehat{\gamma}(z)(\cdot - z)^{-1}\\ -\widehat{\gamma}(z)(\cdot - z)^{-1}\end{pmatrix}.$$

Since

$$\Phi(A_\varkappa - zI)^{-1}\Phi^*P_K\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} = P_K\frac{1}{\cdot - z}\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} \text{ for all } z \in \mathbb{C}_-\,,$$

one has

$$\begin{pmatrix}S^*(\overline{z})\widehat{\gamma}(z)(\cdot - z)^{-1}\\ -\widehat{\gamma}(z)(\cdot - z)^{-1}\end{pmatrix} = 0,$$

which in its turn implies

$$\big(S^* - S^*(\overline{z})\big)\widehat{\gamma}(z)(\cdot - z)^{-1} = 0\,.$$

From this equality, by virtue of the assumption that $\ker(\alpha) = \{0\}$, one obtains that $\gamma(z) = 0$ for all $z \in \mathbb{C}_- \cap \rho(A_\varkappa)$ (see details in the proof of [47, Lemma 4]). Taking into account the definition of $\widehat{\gamma}$, one arrives at

$$\chi_\varkappa^- P_\pm(S\,\widetilde{g} + g) + \chi_\varkappa^+ P_\pm(\widetilde{g} + S^*g) = 0\,.$$

The inclusion

$$\left\{\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} \in \mathfrak{H} : \Phi(A_\varkappa - zI)^{-1}\Phi^*P_K\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} = P_K\frac{1}{\cdot - z}\begin{pmatrix}\widetilde{g}\\ g\end{pmatrix} \text{ for all } z \in \mathbb{C}_+\right\} \subset \mathfrak{N}_+^\varkappa$$

is proved in a similar way.

Proof of Theorem 4.3. To prove the inclusion

$$\widetilde{N}_-^\varkappa \subset \left\{u \in \mathcal{H} : \chi_\varkappa^+\alpha\Gamma_0(A_\varkappa - zI)^{-1}u \in H_-^2(E)\right\},$$

one has to show that $u \in \Phi^* P_K \mathfrak{N}_-^{\varkappa}$ implies $\chi_{\varkappa}^+ \alpha\Gamma_0(A_{\varkappa} - zI)^{-1}u \in H^2_-(E)$. By (25), if $u = \Phi^* P_K \binom{\widetilde{g}}{g}$, then

$$\Phi u = \begin{pmatrix} \widetilde{g} - P_+(\widetilde{g} + S^* g) \\ g - P_-(S\,\widetilde{g} + g) \end{pmatrix}.$$

Thus, in view of the inclusion $\binom{\widetilde{g}}{g} \in K$, it follows from (62) that

$$\begin{aligned} \mathcal{F}_+ u &= \widetilde{g} - P_+(\widetilde{g} + S^* g) + S^* g - S^* P_-(S\widetilde{g} + g) \\ &= (I - P_+)(\widetilde{g} + S^* g) - S^* P_-(S\widetilde{g} + g) \\ &= P_-(\widetilde{g} + S^* g) - S^* P_-(S\widetilde{g} + g)\,. \end{aligned}$$

By analytic continuation of $\mathcal{F}_+ u$ into the lower half-plane, taking into account (60), one arrives at

$$\alpha\Gamma_0(A_{\mathrm{i}I} - zI)^{-1}u = -\sqrt{2\pi}\big(P_-(\widetilde{g} + S^* g)(z) - S^*(\overline{z})P_-(S\widetilde{g} + g)(z)\big) \quad \forall z \in \mathbb{C}_-.$$

Combining this with Lemma 3.1(ii), we write

$$\alpha\Gamma_0(A_{\varkappa} - zI)^{-1}u = -\sqrt{2\pi}\Theta_{\varkappa}^{-1}(z)\big(P_-(\widetilde{g} + S^* g)(z) - S^*(\overline{z})P_-(S\widetilde{g} + g)(z)\big).$$

Finally, using Lemma A.1 from the proof of Theorem 4.2 above, we obtain

$$\chi_{\varkappa}^+ \alpha\Gamma_0(A_{\varkappa} - zI)^{-1}u = \sqrt{2\pi}P_-(S\widetilde{g} + g)(z),$$

To demonstrate the converse inclusion

$$\big\{u \in \mathcal{H} : \chi_{\varkappa}^+ \alpha\Gamma_0(A_{\varkappa} - zI)^{-1}u \in H^2_-(E)\big\} \subset \widetilde{N}_-^{\varkappa},$$

we show that, whenever $\chi_{\varkappa}^+ \alpha\Gamma_0(A_{\varkappa} - zI)^{-1}u \in H^2_-(E)$, the vector

$$\begin{pmatrix} \widetilde{g} \\ g \end{pmatrix} = \Phi u - \frac{1}{2\pi}\begin{pmatrix} 0 \\ \alpha\Gamma_0(A_{\varkappa} - zI)^{-1}u \end{pmatrix}$$

satisfies

$$P_-\left(\chi_{\varkappa}^+(\widetilde{g} + S^* g) + \chi_{\varkappa}^-(S\widetilde{g} + g)\right) = 0,$$

and hence $u = \Phi^* P_K \binom{\widetilde{g}}{g} \in \Phi^* P_K \mathfrak{N}_-^{\varkappa} = \widetilde{N}_-^{\varkappa}$. Indeed, introducing the notation

$$\Phi u =: \begin{pmatrix} \widetilde{g_0} \\ g_0 \end{pmatrix}, \quad h^- := \frac{1}{2\pi}\alpha\Gamma_0(A_{iI} - zI)^{-1}u,$$

we have

$$\begin{aligned} &P_-\left(\chi_{\varkappa}^+(\widetilde{g_0} + S^*(g_0 + h^-)) + \chi_{\varkappa}^-(S\widetilde{g_0} + g_0 + h^-)\right) \\ &\quad = \chi_{\varkappa}^+(\widetilde{g_0} + S^* g_0) - P_+\chi_{\varkappa}^+(\widetilde{g_0} + S^* g_0) \\ &\qquad + P_-\chi_{\varkappa}^-(S\widetilde{g_0} + g_0) + \big(I + \chi_{\varkappa}^+(S^* - I)\big)h^- \\ &\quad = \chi_{\varkappa}^+\mathcal{F}_+ u + \big(I + \chi_{\varkappa}^+(S^* - I)\big)h^-, \end{aligned} \tag{71}$$

By the analytic continuation into the lower half-plane and from Lemma 3.1(i), it follows that (71) represents the boundary value on the real line of the function

$$\begin{aligned} &-\frac{1}{2\pi}\chi_\varkappa^+\alpha\Gamma_0(A_{iI}-zI)^{-1}u+\big(I+\chi_\varkappa^+(S^*(\overline{z})-I)\big)h^-(z) \\ &=-\frac{1}{2\pi}\chi_\varkappa^+\Theta_\varkappa(z)\alpha\Gamma_0(A_\varkappa-zI)^{-1}u+\big(I+\chi_\varkappa^+(S^*(\overline{z})-I)\big)h^-(z) \qquad (72)\\ &=\big(I+\chi_\varkappa^+(S^*(\overline{z})-I)\big)\left(h^-(z)-\frac{1}{2\pi}\chi_\varkappa^+\alpha\Gamma_0(A_\varkappa-zI)^{-1}u\right)=0, \qquad (73)\end{aligned}$$

where in order to pass from (72) to (73), we have used the fact that (see (8))

$$\chi_\varkappa^+\Theta_\varkappa(z)=\big(I-\mathrm{i}\chi_\varkappa^+\alpha(B_{\mathrm{i}I}-M(z))^{-1}\alpha\big)\chi_\varkappa^+=\big(I+\chi_\varkappa^+(S^*(\overline{z})-I)\big)\chi_\varkappa^+, \quad z\in\mathbb{C}_-.$$

Hence, the expression (71) vanishes, which concludes the proof.

The property

$$\widetilde{N}_+^\varkappa=\big\{u\in\mathcal{H}:\chi_\varkappa^-\alpha\Gamma_0(A_\varkappa-zI)^{-1}u\in H_+^2(E)\big\}$$

is proved in a similar way.

Proof of Proposition 5.1**.** Suppose that $z\in\mathbb{C}_+$. If

$$\int_{\mathbb{R}}\frac{d\mu(s)}{s-z}\in H_+^2\,,$$

then, by [58, Theorem 5.19], there exists a function $f\in L^2(\mathbb{R})$ such that

$$\int_{\mathbb{R}}\frac{f(s)ds-d\mu(s)}{s-z}=0\,.$$

Fix a $z_0\in\mathbb{C}_+$, then

$$\begin{aligned} 0=&\int_{\mathbb{R}}\frac{f(s)ds-d\mu(s)}{s-z}-\int_{\mathbb{R}}\frac{f(s)ds-d\mu(s)}{s-z_0}\\ =&(z-z_0)\int_{\mathbb{R}}\frac{f(s)ds-d\mu(s)}{(s-z)(s-z_0)}\,.\end{aligned}$$

Thus, one has

$$\int_{\mathbb{R}}\frac{1}{s-z}\frac{f(s)ds-d\mu(s)}{s-z_0}=0\,,\qquad\text{for all } z\in\mathbb{C}_+\setminus\{z_0\}\,,$$

where now $(s-z_0)^{-1}(f(s)ds-d\mu(s))$ is a complex measure on $\mathbb{R}$. Further, we invoke to the upper half-plane counterpart of the theorem by F. and M. Riesz obtained by applying the conformal mapping from the unit circle onto the upper half plane [34, Chap. 2, Sect. A]. This theorem implies that $(s-z_0)^{-1}(f(s)dt-d\mu(s))$ is absolutely continuous with respect to the Lebesgue measure and, therefore, the same applies to $d\mu(s)$.

The case of H_-^2 is treated likewise.

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Asymptotics of Chebyshev Polynomials, III. Sets Saturating Szegő, Schiefermayr, and Totik–Widom Bounds

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Abstract. We determine which sets saturate the Szegő and Schiefermayr lower bounds on the norms of Chebyshev Polynomials. We also discuss sets that saturate our optimal Totik–Widom upper bound.

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1. Introduction

Let $\mathfrak{e} \subset \mathbb{C}$ be a compact, not finite set. For any continuous, complex-valued function, f, on $\mathfrak{e}$, let

$$\|f\|_{\mathfrak{e}} = \sup_{z\in\mathfrak{e}} |f(z)|. \tag{1.1}$$

The Chebyshev polynomial, T_n, of $\mathfrak{e}$ is the (it turns out unique) degree n monic polynomial that minimizes $\|P\|_{\mathfrak{e}}$ over all degree n monic polynomials, P. We define

$$t_n = \|T_n\|_{\mathfrak{e}}. \tag{1.2}$$

This paper continues our study [3, 4] of t_n and T_n, especially their asymptotics as $n \to \infty$. We let $C(\mathfrak{e})$ denote the logarithmic capacity of $\mathfrak{e}$ (see [18, Sect. 3.6] or [1, 7, 10, 11, 16] for the basics of potential theory).

Szegő [22] proved for all compact $\mathfrak{e} \subset \mathbb{C}$ and all n that

$$t_n \geq C(\mathfrak{e})^n, \tag{1.3}$$

while Schiefermayr [17] proved if $\mathfrak{e} \subset \mathbb{R}$, then

$$t_n \geq 2C(\mathfrak{e})^n. \tag{1.4}$$

This paper had its genesis in a question asked us by J. P. Solovej about which $\mathfrak{e}$ have equality in (1.3) or (1.4). After we found the solution described below, we

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found that for $\mathfrak{e} \subset \mathbb{R}$ the question was answered by Totik [25] using, in part, ideas of Peherstorfer [15] (related ideas appear earlier in Sodin–Yuditskii [20]). Moreover, for a special set of domains in $\mathbb{C}$, it was answered implicitly (without proof) in Totik [26]. We feel it appropriate to publish our proofs because [26] is neither explicit nor comprehensive and mainly because our proofs are different and, we feel, illuminating. In addition, the sets $\mathfrak{f}_n$ which we introduce in Section 3 may be useful in the future. Here are our two main results:

Theorem 1.1 (Totik [25]). *Let $\mathfrak{e} \subset \mathbb{R}$. Fix n. Then $t_n = 2C(\mathfrak{e})^n$ if and only if there is a polynomial, P, of degree n so that*

$$\mathfrak{e} = P^{-1}([-2,2]). \tag{1.5}$$

Remarks. 1. We emphasize that in (1.5), we mean that any $z \in \mathbb{C}$ with $P(z) \in [-2,2]$ has $z \in \mathfrak{e}$ (as well as $P(\mathfrak{e}) = [-2,2]$) not just for $z \in \mathbb{R}$.

2. It is easy to see that T_n is then a multiple of P.

3. In particular, if $t_1 = 2C(\mathfrak{e})$ and $\mathfrak{e} \subset \mathbb{R}$, then $\mathfrak{e}$ is an interval and equality holds in (1.4) for all n. We note that Totik [27, Theorem 3] has a stronger related result. He proves that if $\lim_{n\to\infty} \|T_n\|_{\mathfrak{e}}/C(\mathfrak{e})^n = 2$ for some $\mathfrak{e} \subset \mathbb{R}$, then $\mathfrak{e}$ is an interval.

4. Totik mentions that the ideas in the result and proof are mainly in Peherstorfer [15]. The sets for which equality holds in (1.4) are precisely the sets that Peherstorfer called T-sets and which Sodin–Yuditskii [20] call n-regular sets. They are precisely the spectra of the period n Jacobi matrices which we called period-n sets in [3].

Theorem 1.2. *Let $\mathfrak{e} \subset \mathbb{C}$. Fix n. Then $t_n = C(\mathfrak{e})^n$ if and only if there is a polynomial, P, of degree n with*

$$O\partial(\mathfrak{e}) = P^{-1}(\partial\mathbb{D}) \tag{1.6}$$

where $O\partial$ is the outer boundary and $\mathbb{D}$ the open unit disk.

Remarks. 1. If $\mathfrak{e}$ is compact, then $\mathbb{C} \setminus \mathfrak{e}$ has exactly one unbounded component, $\mathfrak{e}^\sharp$. Its boundary is $O\partial(\mathfrak{e})$. We call $\mathbb{C} \setminus \overline{\mathfrak{e}^\sharp}$ the interior of $O\partial(\mathfrak{e})$ and $\mathfrak{e}^\sharp$ the exterior of $O\partial(\mathfrak{e})$.

2. We'll state several equivalent forms of this theorem in Sect. 3 below.

3. When $\mathfrak{e}$ is a finite union of analytic Jordan curves lying exterior to each other, this result is stated in passing and without proof in Totik [26]. In that case, $O\partial(\mathfrak{e}) = \mathfrak{e}$ so Totik doesn't mention outer boundaries.

4. Polynomial inverse images of $\partial\mathbb{D}$ are called lemniscates (see [21]). We'll say more about their structure in Section 3, but we note that generically they are a union of at most $\deg(P)$ disjoint mutually exterior analytic Jordan curves and in general, a union of at most $\deg(P)$ piecewise analytic Jordan curves with disjoint interiors but with possible intersections at finitely many points.

5. It is easy to see that T_n is a multiple of P.

6. In particular, $t_1 = C(\mathfrak{e})$ if and only if $O\partial(\mathfrak{e})$ is a circle.

It follows from these theorems that if t_n has equality in (1.3) (resp. $\mathfrak{e} \subset \mathbb{R}$ and t_n has equality in (1.4)), then for any $k = 1, 2, \ldots$, t_{nk} also has equality in (1.3) (resp. (1.4)) (by using a suitable scaling of P^k). We want to note that this can be proven directly:

Theorem 1.3. *If t_n has equality in* (1.3)*, then so does t_{nk} for $k = 1, 2, \ldots$*

Proof. Since $(T_n)^k$ is monic, $t_{nk} = \|T_{nk}\|_{\mathfrak{e}} \leq \|(T_n)^k\|_{\mathfrak{e}} = t_n^k = C(\mathfrak{e})^{nk}$ if t_n has equality in (1.3). By Szegő's lower bound, we see that $t_{nk} = C(\mathfrak{e})^{nk}$. □

Theorem 1.4. *If $\mathfrak{e} \subset \mathbb{R}$ and t_n has equality in* (1.4)*, then so does t_{nk} for $k = 1, 2, \ldots$*

Proof. We can't use $(T_n)^k$ since that only leads to $t_{nk} \leq 2^k C(\mathfrak{e})^{nk}$. The key is to realize that $z \mapsto z^k$ is the kth Chebyshev polynomial for $\{z \mid |z| \leq t_n\}$, so we replace $z \mapsto z^k$ by the kth Chebyshev polynomial, S_k, for $\mathfrak{g}_n \equiv [-t_n, t_n]$. Since $C([-t_n, t_n]) = t_n/2$ and equality in (1.4) holds for all n for intervals, we have that $\|S_k\|_{\mathfrak{g}_n} = 2(t_n/2)^k$. Since $S_k \circ T_n$ is a monic polynomial of degree kn, we have that

$$t_{nk} \leq \|S_k \circ T_n\|_{\mathfrak{e}} \leq \|S_k\|_{\mathfrak{g}_n} = 2(2C(\mathfrak{e})^n/2)^k = 2C(\mathfrak{e})^{kn}$$

so, as in the last proof, $t_{nk} = 2C(\mathfrak{e})^{kn}$. □

We prove Theorem 1.1 in Sect. 2, Theorem 1.2 in Sect. 3, consider when the upper bound we found in [3] is optimal in Sect. 4 and discuss related problems in Sects. 5 and 6. JSC and MZ would like to thank Fiona Harrison and Elena Mantovan for the hospitality of Caltech where much of this work was done. We are delighted to dedicate this paper to the memory of Boris Pavlov. One of us (BS) in particular owes Boris a tremendous debt for having sent him talented undergraduates that Boris mentored in St. Petersburg (Kiselev) and Aukland (Killip) who then did doctoral studies at Caltech.

2. The Real Case

In this section, we'll prove Theorem 1.1. Both it and Theorem 1.2 rely on the following simple fact.

Proposition 2.1. *Let $\mathfrak{e} \subset \mathfrak{g}$ be two compact subsets of $\mathbb{C}$ with positive capacity and let $\rho_{\mathfrak{g}}$ (resp. $\rho_{\mathfrak{e}}$) be the potential theoretic equilibrium measure for $\mathfrak{g}$ (resp. $\mathfrak{e}$). Then $C(\mathfrak{e}) = C(\mathfrak{g})$ if and only if $\mathrm{supp}(\rho_{\mathfrak{g}}) \subset \mathfrak{e}$.*

Remark. Section 4 has another proof of this; see Proposition 4.1.

Proof. Let $\mathcal{E}(\mu)$ be the logarithmic potential energy of a finite positive measure, i.e.,

$$\mathcal{E}(\mu) = \iint \log(|x-y|^{-1})\, d\mu(x)d\mu(y) \tag{2.1}$$

so that $\rho_{\mathfrak{g}}$ is the unique probability measure minimizing $\mathcal{E}(\mu)$ among all probability measures with $\operatorname{supp}(\mu) \subset \mathfrak{g}$. Since $C(\mathfrak{e}) = e^{-\mathcal{E}(\rho_{\mathfrak{e}})}$, we have that

$$C(\mathfrak{e}) = C(\mathfrak{g}) \iff \mathcal{E}(\rho_{\mathfrak{e}}) = \mathcal{E}(\rho_{\mathfrak{g}}) \iff \rho_{\mathfrak{e}} = \rho_{\mathfrak{g}} \tag{2.2}$$

for, since $\rho_{\mathfrak{e}}$ is a trial measure for the $\mathfrak{g}$ potential minimum problem and the minimizer is unique, we have that $\mathcal{E}(\rho_{\mathfrak{e}}) \geq \mathcal{E}(\rho_{\mathfrak{g}})$ with equality if and only if $\rho_{\mathfrak{e}} = \rho_{\mathfrak{g}}$.

If $\rho_{\mathfrak{e}} = \rho_{\mathfrak{g}}$, since $\operatorname{supp}(\rho_{\mathfrak{e}}) \subset \mathfrak{e}$, we see that $\operatorname{supp}(\rho_{\mathfrak{g}}) \subset \mathfrak{e}$. Conversely, if $\operatorname{supp}(\rho_{\mathfrak{g}}) \subset \mathfrak{e}$, then $\rho_{\mathfrak{g}}$ is a trial measure for the $\mathfrak{e}$ potential problem and so the minimizer since it is the minimizer for the larger minimization problem. It follows that $\rho_{\mathfrak{e}} = \rho_{\mathfrak{g}}$ so, by (2.2), $C(\mathfrak{e}) = C(\mathfrak{g})$. □

Recall that, given $\mathfrak{e} \subset \mathbb{R}$, in [3], we defined

$$\mathfrak{e}_n = T_n^{-1}([-t_n, t_n]) \tag{2.3}$$

and proved that

$$\mathfrak{e} \subset \mathfrak{e}_n \subset \mathbb{R} \tag{2.4}$$

and

$$t_n = 2C(\mathfrak{e}_n)^n. \tag{2.5}$$

It is also easy to see [3, (2.9)] that if

$$\Delta_n(z) = \frac{2T_n(z)}{t_n} \tag{2.6}$$

then the potential theoretic Green's function for $\mathfrak{e}_n$ is given by

$$G_{\mathfrak{e}_n}(z) = \frac{1}{n} \log \left| \frac{\Delta_n(z)}{2} + \sqrt{\left(\frac{\Delta_n(z)}{2}\right)^2 - 1} \right|. \tag{2.7}$$

This can be shown to imply that the equilibrium measure for $\mathfrak{e}_n$ is [3, Theorem 2.3]

$$d\rho_{\mathfrak{e}_n}(x) = \frac{|\Delta_n'(x)|}{\pi n \sqrt{4 - \Delta_n(x)^2}} \chi_{\mathfrak{e}_n}(x)\, dx \tag{2.8}$$

where $\chi_{\mathfrak{e}_n}$ is the characteristic function of $\mathfrak{e}_n$. Since Δ_n is a polynomial, Δ_n' is non-vanishing on $\mathfrak{e}_n$ except for a possible finite set in $\mathfrak{e}_n$ (which one can specify precisely but we don't need to). We have the following:

Lemma 2.2.

$$\operatorname{supp}(\rho_{\mathfrak{e}_n}) = \mathfrak{e}_n. \tag{2.9}$$

Proof of Theorem 1.1. Since $\mathfrak{e} \subset \mathfrak{e}_n$, by Proposition 2.1, we have that

$$C(\mathfrak{e}) = C(\mathfrak{e}_n) \iff \mathfrak{e}_n = \operatorname{supp}(\rho_{\mathfrak{e}_n}) \subset \mathfrak{e} \iff \mathfrak{e} = \mathfrak{e}_n. \tag{2.10}$$

On the one hand, by (2.5), $t_n = 2C(\mathfrak{e})^n \Rightarrow C(\mathfrak{e}) = C(\mathfrak{e}_n) \Rightarrow \mathfrak{e} = \mathfrak{e}_n \Rightarrow \mathfrak{e} = \Delta_n^{-1}([-2,2])$ so (1.5) holds with $P = \Delta_n$. On the other hand, if (1.5) holds, it is easy to see that $T_n = cP$ and then that $\mathfrak{e}_n = \mathfrak{e}$, so by (2.5), we get equality in (1.4). □

The above proof is only a slight variant of the proof in Totik [25]. We include it mainly to set the stage for the next section.

3. The Complex Case

In this section, we will prove Theorem 1.2. The key to the proof is to define a complex analog of the sets $\mathfrak{e}_n$. We believe that these sets, $\mathfrak{f}_n$, will be useful elsewhere and are the most important idea in this paper. Given a compact set $\mathfrak{e} \subset \mathbb{C}$ and its Chebyshev polynomial, T_n, we define

$$\mathfrak{f}_n = \{z \mid |T_n(z)| \leq t_n\} = T_n^{-1}\big(\{z \mid |z| \leq t_n\}\big). \tag{3.1}$$

Theorem 3.1. *(a)*

$$\mathfrak{e} \subset \mathfrak{f}_n; \tag{3.2}$$

(b)

$$\|T_n\|_{\mathfrak{e}} = t_n = C(\mathfrak{f}_n)^n. \tag{3.3}$$

Remarks. 1. These are analogs of (2.4) and (2.5).

2. They immediately imply (1.3) (not that Szegő's proof [19, Theorem 4.3.7] is very hard) since (3.2)$\Rightarrow C(\mathfrak{f}_n) \geq C(\mathfrak{e})$.

Proof. (a) is trivial.

(b) Let h be defined on $\mathbb{C}$ by

$$h(z) = \begin{cases} 0, & \text{if } |T_n(z)| \leq t_n, \\ \frac{1}{n}\log\left(\frac{|T_n(z)|}{t_n}\right), & \text{if } |T_n(z)| \geq t_n. \end{cases} \tag{3.4}$$

Then h is continuous on $\mathbb{C}$ and harmonic on $\mathbb{C} \setminus \mathfrak{f}_n$ and near infinity has the asymptotics

$$h(z) = \log|z| - \tfrac{1}{n}\log(t_n) + o(1). \tag{3.5}$$

From the first term and $h(z) = 0$ on $\mathfrak{f}_n$, we see that h is the Green's function, $G_{\mathfrak{f}_n}$, for $\mathfrak{f}_n$. By the realization of the capacity in the asymptotics of the Green's function [18, (3.7.4) & (3.7.6)] and (3.5), we see that

$$C(\mathfrak{f}_n) = t_n^{1/n}$$

which is (3.3). □

The proof of (b) just depended on the form of $\mathfrak{f}_n$ and not that, a priori, T_n is a Chebyshev polynomial. We thus can prove (see also [16, Theorem 5.2.5]):

Theorem 3.2. *Let P be a degree n polynomial with*

$$P(z) = cz^n + \cdots \tag{3.6}$$

and let

$$S_\alpha = \{z \mid |P(z)| \leq \alpha\} \tag{3.7}$$

for some $\alpha > 0$. Then

$$C(S_\alpha) = (\alpha/|c|)^{1/n} \tag{3.8}$$

and for S_α, we have $T_n = c^{-1}P$. In particular, S_α obeys

$$\|T_n\|_{S_\alpha} = C(S_\alpha)^n \tag{3.9}$$

Proof. As in the proof of Theorem 3.1, outside of S_α, the Green's function is $\frac{1}{n}\log(|P(z)|/\alpha)$, whose asymptotics at infinity is $\log(|z|) + \frac{1}{n}\log(|c|/\alpha) + \mathrm{o}(1)$ so (3.8) holds.

Note that $Q = c^{-1}P$ is a monic polynomial with $\|Q\|_{S_\alpha} = C(S_\alpha)^n$. By Szegő's lower bound, $\|Q\|_{S_\alpha} \le t_n$ which implies that $Q = T_n$ by the minimum and uniqueness properties of T_n. □

Clearly,

$$\partial S_\alpha = \{z \mid |P(z)| = \alpha\} \equiv L_\alpha. \tag{3.10}$$

This is a *lemniscate* [21]; $|P|$ is C^1 away from the zeros of P and, using the Cauchy–Riemann equations, it is easy to see that if $P(z_0) \neq 0$ then $\nabla|P|(z_0) = 0 \Leftrightarrow P'(z_0) = 0$. Hence the critical values of $|P|$ are precisely those α for which there is a z_0 with $P'(z_0) = 0$ and $|P(z_0)| = \alpha$. At non-critical values, L_α is thus a union of disjoint, mutually exterior, analytic Jordan curves. For α small, the number of curves is exactly the number of distinct zeros of P. As α increases, the number of components changes exactly as α reaches a critical value, α_0, at which point the number of components decreases by the number of critical points (counting multiplicity) on L_{α_0}. At such values, the closure of the components of the non-critical points are piecewise analytic Jordan curves with disjoint interiors and with corners at the critical points. For α large, L_α is a single analytic Jordan curve.

We call S_α, which is the union of the insides of the Jordan curves in L_α, a solid lemniscate. It is easy to describe the equilibrium measure of such sets.

Theorem 3.3. *Fix a degree n polynomial P and $\alpha > 0$. Then*

(a)

$$d\rho \equiv \frac{1}{2\pi i n}\frac{P'(z)}{P(z)}dz \restriction L_\alpha \tag{3.11}$$

is a probability measure;

(b) On L_α, we have that

$$\frac{P'(z)}{P(z)}\,dz = \left|\frac{P'(z)}{P(z)}\right|\,|dz|; \tag{3.12}$$

(c)

$$d\rho = \frac{1}{2\pi n}\frac{d}{|dz|}\mathrm{Arg}(P(z))|dz| \restriction L_\alpha; \tag{3.13}$$

(d) The measure in (3.11) *is the equilibrium measure of S_α;*

(e) $\mathrm{supp}(d\rho) = L_\alpha$.

Remarks. 1. The symbol dz on a curve needs an orientation. We'll specify this orientation in the proof. Basically, it is counter-clockwise around S_α.

2. The proof shows that each Jordan curve in L_α has ρ measure k/n, where k is the number of zeros of P (counting multiplicity) inside that curve.

3. One can also prove the critical (d) by using the formula for the Green's function and by evaluating the normal derivative of $\log(|P|)$ on L_α.

Proof. (a), (b), and (c). Since P has no zeros on L_α, we can locally define an analytic function $W(z) = \log(P(z))$ on each Jordan curve in L_α. Its derivative is $P'(z)/P(z)$ irrespective of which branch of log that we take. Moreover, if locally $P(z) = \alpha e^{i\theta(z)}$ on each such curve and if we parameterize the curve by arc length, $\gamma(s)$, with the curve oriented so that S_α is to the curve's left, then, for z_1 and z_0 nearby points with $z_j = \gamma(s_j)$ where $s_1 > s_0$, we have that $\theta_1 \equiv \theta(z_1) > \theta(z_0) = \theta_0$. This is easy to see using the Cauchy–Riemann equations for $\log(P(z))$ and the fact that its real part increases in the direction outwards from S_α. Moreover, if $d\theta(\gamma(s))/ds$ vanishes at $s = s_0$, since $\operatorname{Re} W(z)$ is constant on γ we conclude that $W'(z_0) = 0 \Rightarrow P'(z_0) = 0$. Thus $d\theta/ds$ is strictly positive except at the critical points which implies that θ is strictly increasing on γ.

Clearly,

$$\int_{z_0}^{z_1} \frac{P'(z)}{P(z)}\, dz = \log\left(\frac{P(z_1)}{P(z_0)}\right) = \log\left(\frac{\alpha e^{i\theta_1}}{\alpha e^{i\theta_0}}\right) = i(\theta_1 - \theta_0),$$

proving that the measure in (3.11) is a positive measure. By the argument principle, n times the integral over L_α is the number of zeros in S_α, so, the measure has total mass 1. This proves (a) and the formula for P'/P in terms of θ' proves (c). The positivity of the measure in (a) proves (b).

(d) Fix $w \in \mathbb{C} \setminus S_\alpha$. Let Γ be a single Jordan curve in L_α and R its interior. Then $\log(z - w)$ is analytic in a neighborhood of $\overline{R}$, so, by the residue calculus and the definition of $d\rho$, if

$$P(z) = c \prod_{j=1}^{n} (z - \zeta_j) \tag{3.14}$$

then

$$\int_\Gamma \log(z - w)\, d\rho(z) = \frac{1}{n} \sum_{\zeta_j \in R} \log(\zeta_j - w).$$

Taking real parts and summing over the Jordan curves, we get

$$\int \log|z - w|\, d\rho(z) = \frac{1}{n} \log(|P(w)|/c), \tag{3.15}$$

which we have seen is the Green's function up to a constant. This implies that $d\rho$ is the equilibrium measure.

(e) We've seen that θ' is positive except on the finite set of critical points so the support is all of L_α. □

The last preliminary we need is

Lemma 3.4. *Fix $\alpha > 0$ and let $\mathfrak{e} \subset S_\alpha$. Then*

$$C(\mathfrak{e}) = C(S_\alpha) \iff L_\alpha \subset \mathfrak{e}. \tag{3.16}$$

Proof. Immediate from Proposition 2.1 and the last theorem. □

Proof of Theorem 1.2. Suppose equality holds in (1.3). Then $C(\mathfrak{e}) = C(\mathfrak{f}_n)$. Let $P = T_n/t_n$ so that $\mathfrak{f}_n = S_{\alpha=1}$. By (3.16), $P^{-1}(\partial\mathbb{D}) \subset \mathfrak{e} \subset P^{-1}(\overline{\mathbb{D}})$. By the second inclusion, $\mathbb{C} \setminus P^{-1}(\overline{\mathbb{D}})$ is contained in the unbounded component of $\mathbb{C} \setminus \mathfrak{e}$. By the first inclusion, we conclude that $O\partial(\mathfrak{e}) = P^{-1}(\partial\mathbb{D})$.

Conversely, by Theorem 3.2, if (1.6) holds, let S_1 be the solid lemniscate associated to P. By (1.6) and the lemma, $C(\mathfrak{e}) = C(S_1)$. By Theorem 3.2, the monic multiple, Q, of P is the Chebyshev polynomial for S_1 and $\|Q\|_{S_1} = C(S_1)^n$. Since $\mathbb{C} \setminus S_1 \subset \mathbb{C} \setminus O\partial(\mathfrak{e})$, we have that $\mathfrak{e} \subset S_1$ and thus $\|Q\|_{\mathfrak{e}} \le \|Q\|_{S_1} = C(\mathfrak{e})^n$. This implies that Q is the Chebyshev polynomial of $\mathfrak{e}$ and that equality holds in (1.3). □

We end this section by exploring some alternate forms and consequences of Theorem 1.2.

Corollary 3.5. *Let $\mathfrak{e}$ be a compact subset of $\mathbb{C}$ so that $\mathbb{C} \setminus \mathfrak{e}$ is connected. Fix n. Then $t_n = C(\mathfrak{e})^n$ if and only if $\mathfrak{e}$ is a solid lemniscate.*

Remark. It is fairly easy to prove Theorem 1.2 from this result.

Proof. By Theorem 1.2, this is equivalent to showing that if $\mathbb{C} \setminus \mathfrak{e}$ is connected and $O\partial(\mathfrak{e}) = L_\alpha$, then $\mathfrak{e} = S_\alpha$. To say that $O\partial(\mathfrak{e}) = L_\alpha$ means that the unbounded component of $\mathbb{C} \setminus \mathfrak{e}$ is $\mathbb{C} \setminus S_\alpha$. If that is so and there is only one component, then $\mathbb{C} \setminus S_\alpha = \mathbb{C} \setminus \mathfrak{e}$ so $\mathfrak{e} = S_\alpha$. □

Here are other equivalences that are easy to check given our earlier arguments.

Theorem 3.6. $t_n = C(\mathfrak{e})^n \iff \partial\mathfrak{f}_n \subset \mathfrak{e}$.

Theorem 3.7. $t_n = C(\mathfrak{e})^n$ *if and only if there is a polynomial, P, and $\alpha > 0$ so that $L_\alpha \subset \mathfrak{e} \subset S_\alpha$.*

4. Equality in a Totik–Widom Upper Bound

In [3], we dubbed an upper bound of the form $\|T_n\|_{\mathfrak{e}} \le QC(\mathfrak{e})^n$ a Totik–Widom bound after Widom [28] and Totik [23] who proved it when $\mathfrak{e} \subset \mathbb{R}$ is a finite gap set. In that paper, we proved that

$$\|T_n\|_{\mathfrak{e}} \le 2\exp(PW(\mathfrak{e}))C(\mathfrak{e})^n \tag{4.1}$$

where $PW(\mathfrak{e}) = \sum_{w\in\mathcal{C}} G_{\mathfrak{e}}(w)$ with $\mathcal{C}$ the set of critical points (in $\mathbb{C}$) of $G_{\mathfrak{e}}$ (when $\mathfrak{e} \subset \mathbb{R}$, they lie in $\mathbb{R}$). PW stands for Parreau–Widom who singled out sets with $PW(\mathfrak{e}) < \infty$ in [14, 29]. We'll call sets that are regular for potential theory and obey this condition, PW sets. Our main goal in this section is to discuss when one has equality in this bound.

Since we want to say something about a formula for $\mathfrak{f}_n$, we recall the proof in a more general context, beginning with

Proposition 4.1. *Let* $\mathfrak{e} \subset \mathfrak{g}$ *be two compact subsets of* $\mathbb{C}$ *with positive capacity and let* $\rho_{\mathfrak{g}}$ *(resp.* $\rho_{\mathfrak{e}}$*) be the potential theoretic equilibrium measure for* $\mathfrak{g}$ *(resp.* $\mathfrak{e}$*). Then*

$$\log\left(\frac{C(\mathfrak{g})}{C(\mathfrak{e})}\right) = \int G_{\mathfrak{e}}(z) d\rho_{\mathfrak{g}}(z). \tag{4.2}$$

Remark. Since $G_{\mathfrak{e}}(z) \geq 0$, this implies that $C(\mathfrak{g}) = C(\mathfrak{e})$ if and only if $G_{\mathfrak{e}}(z) = 0$ for $\rho_{\mathfrak{g}}$-a.e. z in $\mathrm{supp}(\rho_{\mathfrak{g}})$. Since $G_{\mathfrak{e}}(z) = 0 \Rightarrow z \in \mathfrak{e}$ and $G_{\mathfrak{e}}(z) = 0$ for q.e. $z \in \mathfrak{e}$, this happens if and only if $\mathrm{supp}(\rho_{\mathfrak{g}}) \subset \mathfrak{e}$. This gives an alternate proof of Proposition 2.1

Proof. It is well-known [18, Theorem 3.6.8] that near $z = \infty$, we have that $G_{\mathfrak{f}}(z) = \log|z| - \log(C(\mathfrak{f})) + \mathrm{O}(1/z)$. Let $h(z) \equiv G_{\mathfrak{e}}(z) - G_{\mathfrak{g}}(z)$ and note that

$$h(z) = \log\left(\frac{C(\mathfrak{g})}{C(\mathfrak{e})}\right) + \mathrm{O}(1/z) \tag{4.3}$$

near ∞. Thus h is harmonic on $\mathbb{C} \setminus \mathfrak{g}$ and bounded near infinity, so harmonic there. It is known [18, Corollary 3.6.28] that $d\rho_{\mathfrak{g}}$ is not just the equilibrium measure but it is harmonic measure at ∞ in the sense that if $H(z)$ is harmonic and bounded on $(\mathbb{C} \cup \{\infty\}) \setminus \mathfrak{g}$ with q.e. boundary values on $\partial\mathfrak{g}$, then

$$H(\infty) = \int H(z) d\rho_{\mathfrak{g}}(z). \tag{4.4}$$

Taking $H = h$ and noting that q.e., $h \restriction \mathfrak{g} = G_{\mathfrak{e}}$, we get (4.2) from (4.3). □

Theorem 4.2. (a) *For any compact* $\mathfrak{e} \subset \mathbb{R}$*,*

$$\|T_n\|_{\mathfrak{e}} = 2C(\mathfrak{e})^n \exp\left(n \int G_{\mathfrak{e}}(x)\, d\rho_{\mathfrak{e}_n}(x)\right). \tag{4.5}$$

(b) *For any compact* $\mathfrak{f} \subset \mathbb{C}$*,*

$$\|T_n\|_{\mathfrak{f}} = C(\mathfrak{f})^n \exp\left(n \int G_{\mathfrak{f}}(z)\, d\rho_{\mathfrak{f}_n}(z)\right). \tag{4.6}$$

Remark. (a) is from [3]; (b) is new although the proof closely follows the proof of (a) in [3].

Proof. Immediate from (2.5), (3.3) and (4.2). □

The following restates the proof of (4.1) from [3] and answers the question of when equality holds.

Theorem 4.3. (4.1) *holds and if for some* $\mathfrak{e} \subset \mathbb{R}$ *and* n*, we have equality in* (4.1)*, then* $\mathfrak{e}$ *is an interval.*

Proof. The set $\mathfrak{e}_n \setminus \mathfrak{e}$ consists of some number of intervals in the gaps of $\mathfrak{e}$, at most one per gap [3, Theorem 2.4] and $\rho_{\mathfrak{e}_n}$ is a purely a.c. measure [3, Theorem 2.3]. In each gap, K, there is a single critical point, w_K of $G_\mathfrak{e}$ and these are all the critical points. Moreover, in each gap, $G_\mathfrak{e}$ is strictly concave so $G_\mathfrak{e}$ takes its maximum value for the gap exactly at the single point w_K. Moreover, $\rho_{\mathfrak{e}_n}(\mathfrak{e}_n \cap K) \leq 1/n$ [3, Theorem 2.4], so $\int_K G_\mathfrak{e}(x)\,d\rho_{\mathfrak{e}_n} < G_\mathfrak{e}(w_K)/n$ since $d\rho_{\mathfrak{e}_n}$ is absolutely continuous. (4.1) follows by summing over gaps and we only get equality in (4.1) if there are no gaps in $\mathfrak{e}$, i.e., if $\mathfrak{e}$ is a closed interval. □

We can also answer when equality in the upper or lower bound occurs asymptotically along a subsequence. In our paper with Yuditskii [4], we focused on subsequences $\{n_j\}_{j=1}^\infty$ where the zeros of T_{n_j} in gaps had limits. There is at most one zero in each gap, K [3, Theorem 2.3]. Let $\mathcal{G}$ denote the set of all gaps of $\mathfrak{e}$, i.e., bounded components of $\mathbb{R} \setminus \mathfrak{e}$. In [4], we defined what we called a gap collection, a subset $\mathcal{G}_0 \subset \mathcal{G}$ and for each $K \in \mathcal{G}_0$, a point $x_K \in K$. We considered subsequences, T_{n_j}, so that for $K \in \mathcal{G} \setminus \mathcal{G}_0$, as $n_j \to \infty$, either T_{n_j} has no zero in K or the zero goes to the one of the two edges of K and so that for $K \in \mathcal{G}_0$, there is a zero for large n_j which goes to x_K as $n_j \to \infty$. This describes all possible limit points of the set of zeros.

Theorem 4.4. *Fix $\mathfrak{e} \subset \mathbb{R}$, a compact set obeying the PW condition, and a subsequence with an associated limiting zero gap collection, $\mathcal{G}_0$ and $\{x_K\}_{K\in\mathcal{G}_0}$. Then*

$$\lim_{j\to\infty} \|T_{n_j}\|_\mathfrak{e}/C(\mathfrak{e})^{n_j} = 2\exp\left(\sum_{K\in\mathcal{G}_0} G_\mathfrak{e}(x_K)\right). \tag{4.7}$$

Proof. For any $K \in \mathcal{G}$ and any j, define

$$v_j(K) = n_j \int_K G_\mathfrak{e}(x)\,d\rho_{\mathfrak{e}_{n_j}}(x) \tag{4.8}$$

and

$$V(K) = \sup_{x\in K} G_\mathfrak{e}(x) = G_\mathfrak{e}(w_K). \tag{4.9}$$

Since, by the PW hypothesis, $V(K)$ is summable and $v_j(K) \leq V(K)$, the dominated convergence theorem implies that

$$\lim_{j\to\infty} \sum_{K\in\mathcal{G}} v_j(K) = \sum_{K\in\mathcal{G}} \lim_{j\to\infty} v_j(K). \tag{4.10}$$

If $K \in \mathcal{G} \setminus \mathcal{G}_0$, since $\rho_{\mathfrak{e}_{n_j}}(K) \leq 1/n_j$ [3, Theorem 2.4] and $G_\mathfrak{e} \to 0$ at the edges, $v_j(K) \to 0$.

If $K \in \mathcal{G}_0$, by [3, Theorem 5.1], there is for j large a single, exponentially small band of $\mathfrak{e}_{n_j}$ entirely in K with x_K in the band and $\rho_{\mathfrak{e}_{n_j}}(K) = 1/n_j$. It follows that $v_j(K) \to G_\mathfrak{e}(x_K)$. Thus, by (4.10), $\sum_{K\in\mathcal{G}} v_j(K) \to \sum_{K\in\mathcal{G}_0} G_\mathfrak{e}(x_K)$. By (4.5), we get (4.7). □

Corollary 4.5. *Fix $\mathfrak{e} \subset \mathbb{R}$, a compact set obeying the PW condition, and a subsequence with an associated limiting zero gap collection, $\mathcal{G}_0$ and $\{x_K\}_{K\in\mathcal{G}_0}$. Then*

(a) *If $\mathcal{G}_0$ is empty, we have*

$$\lim_{j\to\infty} \|T_{n_j}\|_{\mathfrak{e}}/C(\mathfrak{e})^{n_j} = 2. \tag{4.11}$$

(b) *If $\mathcal{G}_0 = \mathcal{G}$ and, for each K, $x_K = w_K$, the critical point in the gap, we have*

$$\lim_{j\to\infty} \|T_{n_j}\|_{\mathfrak{e}}/C(\mathfrak{e})^{n_j} = 2\exp(PW(\mathfrak{e})). \tag{4.12}$$

In general, we cannot say when there exist any subsequences of the type in the Corollary but can with a few extra assumptions (see the discussion after the example). We can analyze an especially simple case completely.

Example 4.6. Fix $0 < a < b$ and let $\mathfrak{e} = [-b,-a]\cup[a,b]$, a two band set symmetric about 0. Then for n odd, T_n is odd (by uniqueness of the Chebyshev polynomial), so the unique zero in the gap $(-a,a)$ is at $x = 0$ which, by symmetry, is the critical point of $G_{\mathfrak{e}}$ in the gap. Thus the ratio along the odds is given by (4.12).

On the other hand, for n even, T_n is even, so by simplicity of zeros, non-vanishing at 0. Since there is at most one zero in $(-a,a)$, there cannot be any, so $\mathcal{G}_0$ is empty and thus, the ratio along the evens is given by (4.11). In fact, more is true. If

$$P(x) = 2 - \frac{4(x-b)^2}{(a-b)^2}$$

then $\mathfrak{e} = P^{-1}([-2,2])$, so $\|T_{2k}\|_{\mathfrak{e}} = 2C(\mathfrak{e})^{2k}$ for all k and the lower bound is an equality for all even numbers. □

In [4], we discussed limits of $T_n/\|T_n\|_{\mathfrak{e}}$ for $\mathfrak{e} \subset \mathbb{R}$ under a stronger condition than PW called DCT. If $\mathfrak{e}$ has what we called a canonical generator, which holds in a generic sense, then [4, Theorem 5.1] every Blaschke product occurs as a limit point of the normalized Chebyshev polynomials which means one has a limit with any set of simple zeros in any set of gaps. It follows that in this generic DCT case, the set of limit points of $\|T_n\|_{\mathfrak{e}}/C(\mathfrak{e})^n$ is exactly the interval $[2, 2\exp(PW(\mathfrak{e}))]$.

Finite gap sets are always DCT and it is not hard to see that they have a canonical generator in the sense of [4] if and only if the harmonic measures of the bands are rationally independent (except for the trivial relation that they sum to 1). Moreover, it is known (Totik [24]) that for sets with q gaps (which is a $2q+2$ dimensional space described by $a_1 < b_1 < \cdots < a_{q+1} < b_{q+1}$) the condition of rationally independent harmonic measures is satisfied on the compliment of a set of dimension $q+2$ so this rational independence condition is highly generic. We thus have

Theorem 4.7. *Let $\mathfrak{e} \subset \mathbb{R}$ be a set with q gaps so that the harmonic measures of any q of the $q+1$ bands are rationally independent. Then the set of limit points of $\|T_n\|_{\mathfrak{e}}/C(\mathfrak{e})^n$ is exactly the interval $[2, 2\exp(PW(\mathfrak{e}))]$.*

5. On a Theorem of Erdős

For this section, it is useful to define dual Chebyshev polynomials as $D_n \equiv T_n/\|T_n\|_{\mathfrak{e}}$. They are related to Chebyshev polynomials as dual Widom maximizers are related to Widom minimizers, namely among all polynomials, p, of degree n with positive leading coefficient and $\|p\|_{\mathfrak{e}} \leq 1$, they are the one with largest leading coefficient. As such, for any such polynomial, p, one has that $|p(z)| \leq |D_n(z)|$ for $|z|$ large. The question is how large.

In [5], Erdős proved

Theorem 5.1. *Let $\mathfrak{e} = [-1, 1]$. Let p be a degree at most n polynomial with real coefficients and $\|p\|_{\mathfrak{e}} \leq 1$. Then for all $|z| \geq 1$, one has that*

$$|p(z)| \leq |D_n(z)|. \tag{5.1}$$

Our goal in this section is first of all to advertise this result but also to note two results related to this. First of all, we want to note that Erdős' method immediately implies

Theorem 5.2. *Let $\mathfrak{e} \subset \mathbb{R}$ be compact. Let D be the minimum diameter disk containing $\mathfrak{e}$. Let p be a degree at most n polynomial with real coefficients. Then for $z \in \mathbb{C} \setminus D$, one has that*

$$|p(z)| \leq \|p\|_{\mathfrak{e}} |D_n(z)|. \tag{5.2}$$

Remark. If $\alpha = \min_{x \in \mathfrak{e}} x$ and $\beta = \max_{x \in \mathfrak{e}} x$, then D has center $\frac{1}{2}(\alpha + \beta)$ and diameter $\beta - \alpha$.

Theorem 5.3. *Let $\mathfrak{e} \subset \mathbb{C}$ be a solid, degree n, lemniscate. Then* (5.2) *holds for all polynomials p of degree at most n and all $z \in \mathbb{C} \setminus \mathfrak{e}$.*

Remark. This implies that for general compact $\mathfrak{e} \subset \mathbb{C}$, we have

$$|p(z)| \leq \|p\|_{\mathfrak{e}} |D_n(z)| \tag{5.3}$$

for $z \in \mathbb{C} \setminus \mathfrak{f}_n$. Note that in general one cannot replace $z \in \mathbb{C} \setminus \mathfrak{f}_n$ by $z \in \mathbb{C} \setminus \mathfrak{e}$.

Proof of Theorem 5.3. Without loss, we can suppose that $\|p\|_{\mathfrak{e}} = 1$. From Theorem 3.2 we know that $\mathfrak{e} = \{z \,|\, |D_n(z)| \leq 1\}$. Thus all zeros of D_n lie in $\mathfrak{e}$, so $f(z) \equiv p(z)/D_n(z)$ is analytic in $\mathbb{C} \setminus \mathfrak{e}$. It is bounded at ∞, so ∞ is a removable potential singularity. Since $|D_n(z)| = 1$ on $\partial\mathfrak{e}$, we have that $|f(z)| \leq 1$ on $\partial\mathfrak{e}$. By the maximum principle, $|f(z)| \leq 1$ on $\mathbb{C} \cup \{\infty\} \setminus \mathfrak{e}$. □

As for Theorem 5.2, the only difference from Erdős' proof is that he considers the set of zeros of D_n' and ± 1. This is the unique alternating set for D_n when $\mathfrak{e} = [-1, 1]$. In general, the alternating set is not unique but there does exist (see [2, 12, 3]) a set $x_0 < x_1 < \cdots < x_n$ of $n + 1$ distinct points in $\mathfrak{e}$ with

$$D_n(x_j) = (-1)^{n-j}; \quad j = 0, 1, \ldots, n. \tag{5.4}$$

The key fact is geometric:

Lemma 5.4. *Let $w_1 \neq w_2$ both in $\mathbb{C}$. Let D be the open disk with $\{(1-\theta)w_1 + \theta w_2 \,|\, 0 \le \theta \le 1\}$ as diameter. Let $z \notin D$. Then*

$$\operatorname{Re}[(\bar{z} - \overline{w}_1)(z - w_2)] \geq 0. \tag{5.5}$$

Proof. $(\zeta, \xi) \mapsto \operatorname{Re}(\bar{\zeta}\xi)$ is the Euclidean inner product on $\mathbb{C}$ viewed as $\mathbb{R}^2$. Thus (5.5) says the angle between $z - w_1$ and $z - w_2$ is acute or right. It is well known that the set of z where the angle is right is exactly ∂D and that inside D the angle is obtuse and outside acute. □

Proof of Theorem 5.2. (following Erdős [5]) Without loss, we can suppose that $\|p\|_{\mathfrak{e}} = 1$. Let $\{x_j\}_{j=0}^n$ be an alternating set for D_n. For $j = 0, 1, \dots, n$, let

$$\ell_j(z) = \prod_{k \neq j} \frac{z - x_k}{x_j - x_k} \tag{5.6}$$

be the Lagrange interpolation polynomials so that $\ell_j(x_k) = \delta_{jk}$ and thus

$$D_n(z) = \sum_{j=0}^{n} (-1)^{n-j} \ell_j(z); \quad p(z) = \sum_{j=0}^{n} p(x_j)\ell_j(z). \tag{5.7}$$

Let $c_j = \prod_{k \neq j}(x_j - x_k)$ so $(-1)^{n-j}c_j > 0$ since $n - j$ of the $\{x_j - x_k\}_{k \neq j}$ are negative. Then

$$\operatorname{Re}[(-1)^{n-i}\overline{\ell_i(z)}(-1)^{n-j}\ell_j(z)] = \frac{\prod_{k \neq i,j} |z - x_k|^2}{(-1)^{n-i}c_i(-1)^{n-j}c_j} \operatorname{Re}[(\bar{z} - \bar{x}_j)(z - x_i)] \geq 0,$$

by Lemma 5.4. Thus, since $|p(x_j)| \le 1$ and $p(x_j)$ is real,

$$\begin{aligned} |p(z)|^2 &= \operatorname{Re}\Big[\sum_{i,j} \overline{\ell_i(z)}\ell_j(z)\overline{p(x_i)}p(x_j)\Big] \le \sum_{i,j} \big|\operatorname{Re}[\overline{\ell_i(z)}\ell_j(z)]\big| \\ &= \sum_{i,j} \operatorname{Re}[(-1)^{n-i}\overline{\ell_i(z)}(-1)^{n-j}\ell_j(z)] = |D_n(z)|^2. \end{aligned}$$ □

6. Invariance of Widom Factors Under Polynomial Preimages

This final section is connected to the earlier ones, in that it involves polynomial inverse images, but is otherwise unrelated. In the work of Widom [28] on asymptotics of Chebyshev polynomials, a key object is $\|T_n\|_{\mathfrak{e}}/C(\mathfrak{e})^n$, which we, following Goncharov–Hatinoğlu [6], call Widom factors. We want to prove:

Theorem 6.1. *Let $\mathfrak{e} \subset \mathbb{C}$ be a compact set, $P(z)$ a monic polynomial of degree $k \geq 1$, and $\mathfrak{e}_P = P^{-1}(\mathfrak{e}) = \{z \in \mathbb{C} \,|\, P(z) \in \mathfrak{e}\}$. Then for every Chebyshev polynomial T_n of $\mathfrak{e}$, the polynomial $T_n \circ P$ is a Chebyshev polynomial of $\mathfrak{e}_P$ and*

$$\frac{\|T_n\|_{\mathfrak{e}}}{C(\mathfrak{e})^n} = \frac{\|T_n \circ P\|_{\mathfrak{e}_P}}{C(\mathfrak{e}_P)^{nk}}. \tag{6.1}$$

Remark. The first part of this result was also proved in [8] by use of the Kolmogorov criterion (see [9]). Our proof is different.

Lemma 6.2 ([16, Theorem 5.2.5])**.** *Let* $\mathfrak{e} \subset \mathbb{C}$ *be a compact set,* p *a polynomial of degree* $k \geq 1$ *with leading coefficient* $1/\gamma$*, and* $\mathfrak{e}_p$ *as above. Then* $C(\mathfrak{e}_p)^k = |\gamma| C(\mathfrak{e})$*.*

Proof. Let $G_\mathfrak{e}$ and $G_{\mathfrak{e}_p}$ be the Green's functions for $\mathfrak{e}$ and $\mathfrak{e}_p$, respectively. Then $G_{\mathfrak{e}_p} = \frac{1}{k}(G_\mathfrak{e} \circ p)$ since both functions are harmonic on $\mathbb{C} \setminus \mathfrak{e}_p$, zero q.e. on $\partial \mathfrak{e}_p$, and asymptotically $\log |z|$ at infinity. Comparing the constant terms in the asymptotics at infinity yields the claimed result. □

Suppose $p(z)$, $q(z)$ are two polynomials with $k = \deg(p) \geq 1$. The average of q over p is defined by

$$\sigma_{q|p}(z) = \frac{1}{k} \sum_{\{\zeta \,|\, p(\zeta) = p(z)\}} q(\zeta), \tag{6.2}$$

where the values of ζ are repeated according to their multiplicity.

Lemma 6.3 ([13])**.** *The average of* q *over* p *is a polynomial in* p*, in fact,* $\sigma_{q|p} = \hat{q} \circ p$ *for some polynomial* $\hat{q}$ *of degree at most* $\deg(q)/\deg(p)$*.*

Proof. Fix $z \in \mathbb{C}$. Then for all sufficiently large $R > 0$, by the residue calculus,

$$\sigma_{q|p}(z) = \frac{1}{2\pi i \deg(p)} \oint_{|\zeta| = R} \frac{q(\zeta) p'(\zeta)}{p(\zeta) - p(z)} \, d\zeta = \sum_{j=0}^{\infty} \frac{p(z)^j}{2\pi i \deg(p)} \oint_{|\zeta| = R} \frac{q(\zeta) p'(\zeta)}{p(\zeta)^{j+1}} \, d\zeta, \tag{6.3}$$

by picking R so large that $|\zeta| = R \Rightarrow |p(z)| < |p(\zeta)|$. Since, for $j > \deg(q)/\deg(p)$, the integrals are zero (by taking R to ∞), we conclude that $\sigma_{q|p} = \hat{q} \circ p$ with $\deg(\hat{q}) \leq \deg(q)/\deg(p)$. □

Proof of Theorem 6.1. Let Q be a monic polynomial of degree nk. By Lemma 6.3, $\sigma_{Q|P}(z) = \hat{Q} \circ P$ where $\deg(\hat{Q}) \leq n$. In fact, since P is monic of degree k and Q is monic of degree nk it follows from (6.3) that $\hat{Q}$ is monic of degree n. In addition, it follows from the definition of the average that $\|\sigma_{Q|P}\|_{\mathfrak{e}_P} \leq \|Q\|_{\mathfrak{e}_P}$. Thus, $\|T_n \circ P\|_{\mathfrak{e}_P} = \|T_n\|_\mathfrak{e} \leq \|\hat{Q}\|_\mathfrak{e} = \|\sigma_{Q|P}\|_{\mathfrak{e}_P} \leq \|Q\|_{\mathfrak{e}_P}$ so $T_n \circ P$ is the (nk)th Chebyshev polynomial of $\mathfrak{e}_p$.

To get the equality of Widom factors note that $\|T_n\|_\mathfrak{e} = \|T_n \circ P\|_{\mathfrak{e}_P}$ and $C(\mathfrak{e}_P)^k = C(\mathfrak{e})$ by Lemma 6.2. □

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Solvability and complex limit bicharacteristics

Nils Dencker

To the memory of Boris Pavlov

Abstract. We shall study the solvability of pseudodifferential operators which are not of principal type. The operator will have complex principal symbol satisfying condition (Ψ) and we shall consider the limits of semibicharacteristics at the set where the principal symbol vanishes of at least second order. The convergence shall be as smooth curves, and we shall assume that the normalized complex Hamilton vector field of the principal symbol over the semicharacteristics converges to a real vector field. Also, we shall assume that the linearization of the real part of the normalized Hamilton vector field at the semibicharacteristic is tangent to and bounded on the tangent space of a Lagrangean submanifold at the semibicharacteristics, which we call a grazing Lagrangean space. Under these conditions one can invariantly define the imaginary part of the subprincipal symbol. If the quotient of the imaginary part of the subprincipal symbol with the norm of the Hamilton vector field switches sign from   to $+$ on the bicharacteristics and becomes unbounded as they converge to the limit, then the operator is not solvable at the limit bicharacteristic.

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1. Introduction

We shall consider the solvability for a classical pseudodifferential operator P on a C^∞ manifold X which is not of principal type. P is solvable at a compact set $K \subseteq X$ if the equation

$$Pu = v \tag{1.1}$$

has a local solution $u \in \mathcal{D}'(X)$ in a neighborhood of K for any $v \in C^\infty(X)$ in a set of finite codimension.

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The pseudodifferential operator P is classical if it has an asymptotic expansion $p_m + p_{m-1} + \cdots$ where p_k is homogeneous of degree k in ξ and $p_m = \sigma(P)$ is the principal symbol of the operator. P is of principal type if the Hamilton vector field

$$H_p = \sum_{j=1}^{n} \partial_{\xi_j} p \partial_{x_j} - \partial_{x_j} p \partial_{\xi_j} \tag{1.2}$$

of the principal symbol $p = p_m$ does not have the radial direction $\langle \xi, \partial_\xi \rangle$ at $p^{-1}(0)$, in particular $H_p \neq 0$ then. By homogeneity H_p is well defined on the cosphere bundle $S^*X = \{ (x,\xi) \in T^*X : |\xi| = 1 \}$, defined by some choice of Riemannean metric, and the principal type condition means that H_p is not degenerate on S^*X. For pseudodifferential operators of principal type, it is known from [1] and [4] that local solvability is equivalent to condition (Ψ):

$$\begin{aligned} &\operatorname{Im}(ap) \text{ does not change sign from } - \text{ to } + \\ &\text{along the oriented bicharacteristics of } \operatorname{Re}(ap) \end{aligned} \tag{1.3}$$

for any $0 \neq a \in C^\infty(T^*M)$. This condition is of course trivial if the principal symbol is real valued. The oriented bicharacteristics are the positive flow-outs of the Hamilton vector field $H_{\operatorname{Re}(ap)} \neq 0$ on $\operatorname{Re}(ap) = 0$, and these are called semibicharacteristics of p.

We shall consider the case when P is not of principal type, instead the complex valued principal symbol vanishes of at least second order at the double characteristics Σ_2. We shall study necessary conditions for solvability when Σ_2 is an involutive manifold, and since solvability is an open condition we shall assume that P satisfies condition (Ψ) in the complement of Σ_2 where it is of principal type. Naturally, condition (Ψ) is empty on Σ_2, where instead we shall have necessary conditions on the next lower term p_{m-1}, called the *subprincipal symbol.* The sum of the principal symbol and subprincipal symbol is called the *refined principal symbol.*

Mendoza and Uhlman [6] studied the case when principal symbol p is a product of two real symbols having transversal Hamilton vector fields at the involutive intersection Σ_2 of the characteristics. They proved that P is not solvable if the subprincipal symbol changes sign on the integral curves of these Hamilton vector fields on Σ_2, which are the limits of the bicharacteristics at Σ_2. Mendoza [7] generalized this to the case when the principal symbol is real and vanishes of second order at an involutive manifold Σ_2 having an indefinite Hessian with rank equal to the codimension of the manifold. The Hessian then gives well-defined limit bicharacteristics over Σ_2, and P is not solvable if the subprincipal symbol changes sign on any of these limit bicharacteristics. Since Σ_2 is involutive, the limits of the bicharacteristics are tangent to the symplectic foliation of Σ_2, see Example 2.6. Thus, both [6] and [7] have constant sign of the subprincipal symbol on the limit characteristics as a necessary condition for solvability, which corresponds to condition (P) on the refined principal symbol. This is natural since when the principal symbol vanishes of exactly second order one gets both directions on the limit bicharacteristics.

These results were generalized in [2] to pseudodifferential operators with real principal symbol for which the linearization of the Hamilton vector field is tangent to and has uniform bounds on the tangent spaces of some Lagrangean manifolds at the bicharacteristics. Then P is not solvable if condition (Ψ) is not satisfied on the limit bicharacteristics, in the sense that the imaginary part of the subprincipal symbol switches sign from $-$ to $+$ on the semibicharacteristics when converging to the limit semibicharacteristic. The paper [3] studied operators of subprincipal type, where the principal symbol vanishes of at least second order at a nonradial involutive manifold Σ_2 and the subprincipal symbol is of principal type with Hamilton vector field tangent to Σ_2 at the characteristics, but transversal to the symplectic foliation of Σ_2. Then the operator was not solvable if the subprincipal symbol is constant on the symplectic leaves of Σ_2 after multiplication with a non-vanishing factor and does not satisfy condition (Ψ) on Σ_2. In fact, if the principal symbol is proportional to a real symbol, then the result of [2] gives nonsolvability in general when the subprincipal symbol is not constant on the leaves.

In this paper, we shall extend the results of [2] to pseudodifferential operators with complex principal symbols. We shall consider the limits of semibicharacteristics at the set Σ_2 where the principal symbol vanishes of at least second order. The convergence shall be as smooth curves, then the limit semibicharacteristic also is a smooth curve. We shall assume that the normalized complex Hamilton vector field of the principal symbol on the semicharacteristics converges to a real vector field on Σ_2. Then the limit semibicharacteristic are uniquely defined, and one can invariantly define the imaginary part of the subprincipal symbol. Also, we shall assume that the linearization of the real part of the normalized Hamilton vector field is tangent to and uniformly bounded on the tangent space of a Lagrangean submanifold at the semibicharacteristics, which we call a grazing Lagrangean space, see (2.8). We shall also assume uniform bounds on linearization of the imaginary part of the Hamilton vector field on the grazing Lagrangean space, see (2.11), (2.13) and Definition 2.3.

Our main result is Theorem 2.11, which essentially says that under these conditions the operator is not solvable at the limit semibicharacteristic if the quotient of the imaginary part of the subprincipal symbol with the norm of the Hamilton vector field switches sign from $-$ to $+$ on the semibicharacteristics and becomes unbounded as they converge to the limit semibicharacteristic, see (2.20). Thus a non-homogeneous version of condition (Ψ) on the refined principal symbol does not hold on the limit characteristics. This result implies the results of [2], [6] and [7].

2. Statement of results

Let p be the principal symbol, $\Sigma = p^{-1}(0)$ be the characteristics, and Σ_2 be the set of double characteristics, i.e., the points on Σ where $dp = 0$. Since we are going to study necessary conditions for solvability, we shall assume that P satisfies condition (Ψ) given by (1.3) on $\Sigma_1 = \Sigma \setminus \Sigma_2$. We shall study limits at Σ_2 of semibicharacteristics, and we shall assume that the normalized limit of H_p is proportional to a real vector field, in the sense that

$$|dp \wedge d\overline{p}| \ll |dp| \quad \text{on } \Gamma_j \text{ as } j \to \infty. \tag{2.1}$$

We shall only use semibicharacteristics given by $H_{\operatorname{Re} ap}$ such that $|\operatorname{Re} a\nabla p| \ge c|\nabla p|$ at Γ_j for some $c > 0$, where ∇p is the gradient of p. Let $\{\Gamma_j\}_{j=1}^\infty$ be a set of semibicharacteristics of p on $S^*X \cap \Sigma_1$ so that Γ_j are bicharacteristics of $\operatorname{Re} a_j p$ where $0 \ne a_j \in C^\infty$ uniformly at Γ_j and

$$|\operatorname{Re} a_j \nabla p| \ge c|\nabla p| \quad \text{at } \Gamma_j \tag{2.2}$$

for some fixed $c > 0$, observe that $p = 0$ on Γ_j. We shall assume that Γ_j are uniformly bounded in C^∞ when parametrized on a uniformly bounded interval (for example, with respect to the arc length). The bounds are defined with respect to some choice of Riemannean metric on S^*X, but different choices of metric will only change the constants. In particular, we have a uniform bound on the arc lengths:

$$|\Gamma_j| \le C \quad \forall\, j. \tag{2.3}$$

In fact, we have that $\Gamma_j = \{\gamma_j(t) :\ t \in I_j\}$ with $|\gamma_j'(t)| \equiv 1$ and $|I_j| \le C$, then $|\gamma_j^{(k)}(t)| \le C_k$ for $t \in I_j$ and $\forall\ j,\ k \ge 1$. Let the normalized gradient $\widetilde{p} = p/|\nabla p|$ and the normalized Hamilton vector field

$$H_{\widetilde{p}} = |H_p|^{-1} H_p \quad \text{on } p^{-1}(0) \setminus \Sigma_2.$$

Then Γ_j is uniformly bounded in C^∞ if there exists positive constants c and C_k such that

$$|H^k_{\operatorname{Re} a_j \widetilde{p}} \nabla \operatorname{Re} a_j \widetilde{p}| \le C_k \quad \text{and} \quad |H_{\operatorname{Re} a_j \widetilde{p}}| \ge c \quad \text{at } \Gamma_j \ \ \forall\, j, k, \tag{2.4}$$

which implies that $|a_j| \ge c > 0$ at Γ_j. This means that the normalized Hamilton vector field $H_{\operatorname{Re} a_j \widetilde{p}}$ is uniformly bounded in C^∞ as a non-degenerate vector field over Γ, and this only depends on $a_j\big|_{\Gamma_j}$. Observe that the semibicharacteristics have a natural orientation given by the Hamilton vector field. Now the set of semicharacteristic curves $\{\Gamma_j\}_{j=1}^\infty$ is uniformly bounded in C^∞ when parametrized with respect to the arc length, and therefore it is a precompact set. Thus there exists a subsequence Γ_{j_k}, $k \to \infty$, that converge to a smooth curve Γ (possibly a point), called a limit semibicharacteristic by the following definition, which generalizes the definition in [2].

Definition 2.1. *We say that a sequence of smooth curves Γ_j on a smooth manifold converges to a smooth limit curve Γ (possibly a point) if there exist parametrizations on uniformly bounded intervals that converge in C^∞. If $p \in C^\infty(T^*X)$, then we say that $\{\Gamma_j\}_{j=1}^\infty$ are a uniform family of semibicharacteristics of p if* (2.3) *and* (2.4) *hold. A smooth curve $\Gamma \subset \Sigma_2 \cap S^*X$ is a* limit semibicharacteristic *of p if there exists a uniform family of semibicharacteristics of p that converge to it.*

Naturally, this definition is invariant under symplectic changes of coordinates, and the set $\{\Gamma_j\}_{j=1}^{\infty}$ may have subsequences converging to several different limit semibicharacteristics, which could be points. For example, if Γ_j is parametrized with respect to the arc length on intervals I_j such that $|I_j| \to 0$, then we find that Γ_j converges to a limit curve which is a point. Observe that if Γ_j converge to a limit semibicharacteristic Γ, then (2.3) and (2.4) must hold for Γ_j.

Example 2.2. Let Γ_j be the curve parametrized by

$$[0,1] \ni t \mapsto \gamma_j(t) = (t, \cos(jt)/j, \sin(jt)/j)/\sqrt{2}.$$

Since $|\gamma_j'(t)| = 1$, the curves are parametrized with respect to arc length, and we have that $\Gamma_j \to \Gamma = \left\{ (t,0,0) : t \in \left[0, 2^{-1/2}\right] \right\}$ in C^0, but not in C^∞ since $|\gamma_j''(t)| = j/\sqrt{2}$. If we parametrize Γ_j with $x = jt \in [0,j]$ we find that Γ_j converge to Γ in C^∞ but not on uniformly bounded intervals.

But we shall also need a condition on the differential of the Hamilton vector field H_p at the semibicharacteristic Γ along a Lagrangean space, which will give bounds on the curvature of the semicharacteristics in these directions. If the semicharacteristics is the bicharacteristic of $\operatorname{Re} ap$ then we shall denote $\Sigma = (\operatorname{Re} ap)^{-1}(0)$ and $T_w\Sigma = \operatorname{Ker} d \operatorname{Re} ap(w) \subset T(T^*X)$, where $d \operatorname{Re} ap(w) \neq 0$ for $w \in \Gamma$. A section of Lagrangean spaces L over a bicharacteristic Γ is a map

$$\Gamma \ni w \mapsto L(w) \subset T_w(T^*X)$$

such that $L(w)$ is a Lagrangean space in $T_w\Sigma$, $\forall\, w \in \Gamma$. If the section L is C^1 then it has tangent space $TL \subset T_L(T_\Gamma(T^*X))$. Observe that since $L(w) \subset T_w\Sigma$ is Lagrangean we find $d \operatorname{Re} ap(w)\big|_{L(w)} = 0$ and $H_{\operatorname{Re} ap}(w) \in L(w)$ when $w \in \Gamma$. Now we shall also have the condition that the *linearization* of $H_{\operatorname{Re} ap}$ at Γ is tangent to the Lagrangean space L.

Definition 2.3. *Let Γ be a semibicharacteristic of p, i.e., a bicharacteristic of* $\operatorname{Re}(ap)$ *for some $0 \neq a \in C^\infty$. We say that a C^1 section of Lagrangean spaces L over Γ is a section of* grazing Lagrangean spaces *of Γ if*

$$L \subset T_\Gamma\Sigma = \operatorname{Ker} d \operatorname{Re} ap\big|_\Gamma \subset T_\Gamma(T^*X),$$

and the linearization (or first order jet) of $H_{\operatorname{Re} ap} \subset T_\Gamma L$, the tangent space of L at Γ.

The linearization of $H_{\operatorname{Re} ap}(w)$ is given by the second order Taylor expansion of $\operatorname{Re} ap$ at w and since $L(w)$ is Lagrangean we find that terms in that expansion that vanish on $L(w)$ have Hamilton field parallel to L. Thus, the condition that the linearization of $H_{\operatorname{Re} ap}(w)$ is in $TL(w)$ only depends on the restriction to $L(w)$ of the second order Taylor expansion of $\operatorname{Re} ap$ at w. We find that Definition 2.3 is invariant under multiplication of $\operatorname{Re} ap$ by nonvanishing real factors because $\operatorname{Re} ap(w) = 0$ and $d \operatorname{Re} ap(w)\big|_{L(w)} = 0$ since $L \subset T_\Gamma\Sigma$. Thus the linearization of $H_{\operatorname{Re} cap}$ is determined by $\operatorname{Hess} \operatorname{Re} cap(w)\big|_{L(w)} = c \operatorname{Hess} \operatorname{Re} ap(w)\big|_{L(w)}$ when c is real. Thus the linearization only depends on the argument of a_j at Γ_j so we can replace $H_{\operatorname{Re} ap}(w)$ by $H_{\operatorname{Re} a\widetilde{p}}$ in the definition.

By Definition 2.3 we find that the linearization of $H_{\operatorname{Re} ap}$ gives an evolution equation for the section L, see Example 2.4. Choosing a Lagrangean subspace of $T_{w_0}\Sigma$ at $w_0 \in \Gamma$ then determines L along Γ, so L must be smooth. Actually, L is the tangent space at Γ of a smooth Lagrangean submanifold of $(\operatorname{Re} ap)^{-1}(0)$, see (3.30).

Example 2.4. Let

$$p = \tau + ia(t,x)\xi_1 - \left(\langle A(t,x)x,x\rangle + 2\langle B(t,x)x,\xi\rangle + \langle C(t,x)\xi,\xi\rangle\right)/2, \ (x,\xi) \in T^*\mathbf{R}^n,$$

where $a(t,x) \in C^\infty$ is real valued, $A(t,x)$, $B(t,x)$ and $C(t,x) \in C^\infty$ are $n \times n$ matrices such that $A(t,x) = A^t(t,x)$ and $C(t) = C^t(t,x)$ are symmetric, and let $\Gamma = \{\, (t,0,0,\xi_0) : \ t \in I \,\}$. Then $H_{\operatorname{Re} p} = \partial_t$ at Γ and

$$(\operatorname{Re} p)^{-1}(0) = \{\, \tau = \langle \operatorname{Re} A(t,x)x,x\rangle/2 + \langle \operatorname{Re} B(t,x)x,\xi\rangle + \langle \operatorname{Re} C(t,x)\xi,\xi\rangle/2 \,\}$$

where $\operatorname{Re} F$ is the given by the real part of the elements of F. The linearization of the Hamilton field H_p at $(t,0,0,\xi_0)$ is

$$\partial_t + ia(t,0)\partial_{x_1} + \langle A(t,0)y + B^t(t,0)\eta, \partial_\eta\rangle - \langle B(t,0)y + C(t,0)\eta, \partial_y\rangle \tag{2.5}$$

with $(y,\eta) \in T(T^*\mathbf{R}^n)$. Since $d\operatorname{Re} p = d\tau$ at Γ, a C^1 section of Lagrangean spaces $L(t) \subset T_\Gamma\Sigma$ must be tangent to Γ. Thus, by choosing linear symplectic coordinates (y,η) we may obtain that

$$L(t) = \{\, (s,y,0,E(t)y) : (s,y) \in \mathbf{R}^n \,\}$$

where $E(t) \in C^1$ is real and symmetric with $E(0) = 0$. By applying (2.5) on $\eta - E(t)y$, which vanishes on $L(t)$, we obtain that $L(t)$ is a grazing Lagrangean space if

$$\partial_t E(t) = \operatorname{Re} A(t,0) + \operatorname{Re} B(t,0)E(t) + E(t)\operatorname{Re} B^t(t) + E(t)\operatorname{Re} C(t,0)E(t). \tag{2.6}$$

Then by uniqueness we find that $L(t)$ is constant in t if and only if $\operatorname{Re} A(t,0) \equiv 0$, and then $A(t,0) = \operatorname{Hess} p\big|_{L(t)}$. In general, the real part of $\operatorname{Hess} p\big|_{L(t)}$ is given by the right hand side of (2.6).

Example 2.5. If p is of principal type, then one can choose $a \neq 0$ and symplectic coordinates so that $\operatorname{Re} ap = \tau$ near $\Gamma = \{\, (t,0,0,\xi_0) : \ t \in I \,\}$. Then one can take any Lagrangean plane in $\operatorname{Ker} d\tau\big|_\Gamma = T_\Gamma\Sigma$ which is tangent to Γ.

Observe that we may choose symplectic coordinates $(t,x;\tau,\xi)$ so that $\tau = \operatorname{Re} ap$ and the fiber of $L(w)$ is equal to $\{\, (s,y,0,0) : (s,y) \in \mathbf{R}^n \,\}$ at $w \in \Gamma = \{\, (t,0;0,\xi_0) : \ t \in I \,\}$. But it is not clear that we can do that *uniformly* for a family of semibicharacteristics $\{\, \Gamma_j \,\}$, for that we need additional conditions. We shall assume that there exists a grazing Lagrangean space L_j of Γ_j, $\forall\, j$, such that the normalized Hamilton vector field $H_{\widetilde{p}}$ satisfies

$$\left| dH_{\widetilde{p}}(w)\big|_{L_j(w)} \right| \le C \quad \text{for } w \in \Gamma_j \ \ \forall\, j. \tag{2.7}$$

This is equivalent to

$$\left| dH_p(w)\big|_{L_j(w)} \right| \le C|H_p| \tag{2.8}$$

for $w \in \Gamma_j$ since $L \subset T_\Gamma\Sigma$. In fact, we have that $dH_{bp} = dbH_p + bdH_p + dpH_b$ on Σ. Since the mapping $\Gamma_j \ni w \mapsto L_j(w)$ is determined by the linearization of $H_{\operatorname{Re} a_j\widetilde{p}}$ on L_j, thus by $dH_{\operatorname{Re} a_j\widetilde{p}}(w)\big|_{L_j(w)}$, condition (2.7) implies that $\Gamma_j \ni w \mapsto L_j(w)$ is uniformly in C^1, see Example 2.4. Observe that condition (2.4) gives (2.7) in the direction of $T_w\Gamma_j \subset L_j(w)$. Clearly condition (2.7) is invariant under changes of symplectic coordinates and multiplications with non-vanishing real factors. In general, we only have $dH_{\widetilde{p}} = \mathcal{O}(|H_p|^{-1})$ since $dH_p = \mathcal{O}(1)$, and by induction we find $\partial^\alpha H_{\widetilde{p}} = \mathcal{O}(|H_p|^{-|\alpha|})$, see Proposition 3.1.

Observe that condition (2.7) gives

$$\left| d\nabla \operatorname{Re} a_j\widetilde{p}(w)\big|_{L_j(w)} \right| \le C \quad \text{for } w \in \Gamma_j \ \ \forall\, j. \tag{2.9}$$

Since $\nabla \operatorname{Re} a_j\widetilde{p}$ is uniformly proportional to the normal of the level surface

$$(\operatorname{Re} a_j p)^{-1}(0),$$

condition (2.9) gives a uniform bound on the curvature of this surface in the directions given by L_j over Γ_j.

Example 2.6. Assume that $p(x,\xi)$ is vanishing of exactly order $k \ge 2$ at the involutive submanifold $\Sigma_2 = \{\, \xi' = 0 \,\}$, $\xi = (\xi', \xi'') \in \mathbf{R}^m \times \mathbf{R}^{n-m}$ such that the localization

$$\eta \mapsto \sum_{|\alpha|=k} \partial_{\xi'}^\alpha p(x,0,\xi'')\eta^\alpha$$

is of principal type if $\eta \ne 0$. Then the semibicharacteristics of p with $|\operatorname{Re} a_j \nabla\widetilde{p}| \cong 1$ satisfies (2.4) and (2.7) with $L_j = \{\, \xi = 0 \,\}$ at any point. In fact, $|\partial_{\xi'} p(x,\xi)| \cong |\xi'|^{k-1}$ and $\partial_{x,\xi''} p(x,\xi) = \mathcal{O}(|\xi'|^k)$ so

$$H_{\widetilde{p}} = \partial_{\xi'}\widetilde{p}\,\partial_{x'} + \mathcal{O}(|\xi'|) \quad \text{and} \quad \partial_x^\alpha \nabla p = \mathcal{O}(|\xi'|^{k-1}) \ \forall\, \alpha,$$

when $|\xi'| \ll 1$ and $|\xi| \cong 1$.

Now for a uniform family of semibicharacteristics $\{\, \Gamma_j \,\}$ we shall denote

$$0 < \min_{\Gamma_j} |H_p| = \kappa_j \to 0 \quad \text{as } j \to \infty, \tag{2.10}$$

and we shall assume that

$$|dp \wedge d\overline{p}\,| \le C\kappa_j^{14/3}|H_p|^2 \quad \text{at } \Gamma_j, \tag{2.11}$$

which by Leibniz' rule means that $|d \operatorname{Re}\widetilde{p} \wedge d \operatorname{Im}\widetilde{p}| \le C\kappa_j^{14/3}$ on Γ_j. In fact, we have

$$d(ap) \wedge d(\overline{ap}) = |a|^2 dp \wedge d\overline{p} + 2i \operatorname{Im}(a\overline{p}\, dp \wedge d\overline{a}) + |p|^2 da \wedge d\overline{a} \tag{2.12}$$

where the two last terms vanish on Σ. This gives a measure on the complex part of H_p and gives that $H_{\widetilde{p}}$ is proportional to a real vector field on Γ_j modulo terms that are $\mathcal{O}(\kappa_j^{14/3})$.

With L_j as in (2.7) we shall assume the following condition

$$\left| d\big|_{L_j}(dp \wedge d\overline{p})(w) \right| \le C\kappa_j^{4/3}|H_p|^2 \quad \text{for } w \in \Gamma_j \quad \forall\, j, \tag{2.13}$$

where the outer differential is restricted to L_j on Γ_j. Observe that condition (2.13) gives an estimate on the variation of the complex part of the Hamilton vector field along L, whereas condition (2.7) gives an estimate on the variation of the Hamilton vector field. Using (2.8), (2.11) and (2.12) we find that (2.13) is equivalent to

$$\left| d\big|_{L_j}(d\,\mathrm{Re}\,\widetilde{p} \wedge d\,\mathrm{Im}\,\widetilde{p})(w) \right| \le C\kappa_j^{4/3} \quad \text{for } w \in \Gamma_j \quad \forall\, j. \tag{2.14}$$

In fact, the differential of the two last terms in (2.12) vanish since $p = 0$ on Γ_j and if $a = |\nabla p|^{-1}$ then $da\big|_{L_j} = \mathcal{O}(a)$ by (2.8).

If $|\nabla\,\mathrm{Re}\,\widetilde{p}\,| \cong |\nabla \widetilde{p}\,| = 1$, then we find from (2.11) that

$$|d\,\mathrm{Im}\,\widetilde{p}(w)| \le C\kappa_j^{14/3} \qquad \text{on } \mathrm{Ker}\, d\,\mathrm{Re}\,\widetilde{p}(w) \tag{2.15}$$

for $w \in \Gamma_j$. Since $d\big|_{L_j} d\,\mathrm{Re}\,\widetilde{p}(w) = \mathcal{O}(1)$ by (2.7), we find from (2.14) that

$$d\big|_{L_j} d\,\mathrm{Im}\,\widetilde{p}(w) = \mathcal{O}(\kappa_j^{4/3}) \qquad \text{on } \mathrm{Ker}\, d\,\mathrm{Re}\,\widetilde{p}(w) \tag{2.16}$$

when $w \in \Gamma_j$. The estimates (2.15) and (2.16) will be needed in order to handle the imaginary part of the principal symbol as a perturbation, see Lemmas 5.1 and 5.2.

Now, since the semibicharacteristics Γ_j are uniform we have $|H_{\mathrm{Re}\, a_j \widetilde{p}}| \ge c$, which by (2.11) gives

$$\mathrm{Im}(a_j \nabla \widetilde{p}) = \beta_j\, \mathrm{Re}(a_j \nabla \widetilde{p}) + V_j \quad \text{at } \gamma_j \tag{2.17}$$

where $\beta_j = \mathcal{O}(1)$ and $|V_j| \le C\kappa_j^{14/3}$. The first part of the right hand side will not change the direction of Γ_j. Thus multiplying $\widetilde{p}$ with the complex factor $1 - i\beta_j$ only changes the direction of the real part of the Hamilton vector field by terms that are $\mathcal{O}\big(\kappa_j^{14/3}\big)$. This only perturbs Γ_j so that the distance to the original semibicharacteristic is $\mathcal{O}(\kappa_j^{14/3})$. Now the derivative of the linearization of the Hamilton vector field is $\mathcal{O}\big(|H_p|^{-1}\big) = \mathcal{O}\big(\kappa_j^{-1}\big)$, see Proposition 3.1. Thus, the linearization is changed with a bounded factor and terms that are $\mathcal{O}\big(\kappa_j^{8/3}\big)$. Thus, we find from (2.6) that the grazing Lagrangean spaces L_j are only changed by terms that are $\mathcal{O}\big(\kappa_j^{8/3}\big)$. Since $\kappa_j \le |H_p|$ on Γ_j we find that conditions (2.8), (2.11) and (2.13) are not changed. Observe that a_j is only defined on Γ_j, but since Γ_j is a uniformly bounded smooth curve, a_j can easily be uniformly extended to a neighborhood of Γ_j.

Remark 2.7. The family of uniform semibicharacteristics $\{\,\Gamma_j\,\}_j$ satisfying condition (2.11) and the grazing Lagrangean spaces L_j of Γ_j are invariant modulo perturbations of $\mathcal{O}(\kappa_j^{14/3})$ under different choices of a_j in (2.4). Thus conditions (2.8), (2.11) and (2.13) are well defined.

Thus, the choice of a_j will be irrelevant when taking the limit. Now, we shall only consider semibicharacteristics Γ_j with tangent vectors $H_{\operatorname{Re} a_j \widetilde{p}}$ so that

$$|H_{\operatorname{Im} a_j \widetilde{p}}| \le C\kappa_j^{14/3} \quad \text{and } |a_j| > 1/C \text{ on } \Gamma_j \tag{2.18}$$

which implies that $|\operatorname{Re} \nabla a_j \widetilde{p}| \ge c > 0$ when $\kappa_j \ll 1$. Then the multipliers a_j are *well defined* on Γ_j modulo uniformly bounded factors which have argument that are $\mathcal{O}(\kappa_j^{14/3})$.

The invariant subprincipal symbol p_s will be important for the solvability of the operator near Σ_2. For the usual Kohn–Nirenberg quantization of pseudodifferential operators, the next lower order term is equal to

$$p_s = p_{m-1} - \frac{1}{2i} \sum_j \partial_{\xi_j} \partial_{x_j} p \tag{2.19}$$

and for the Weyl quantization it is p_{m-1}. Both of these are equal to p_{m-1} at the involutive manifold $\Sigma_2 = \{\, \xi' = 0 \,\}$ since then $\partial_\xi p \equiv 0$ at Σ_2.

For the subprincipal symbol p_s we shall have a condition that essentially means that condition (Ψ) does not hold for the subprincipal symbol. Observe that if (2.18) holds then the imaginary part of $a_j p_s$ is well defined modulo terms that are $\mathcal{O}(\kappa_j^{14/3})$. Assuming (2.18) we shall as in [2] assume that

$$\min_{\partial \Gamma_j} \int \operatorname{Im} a_j p_s |H_p|^{-1} \, ds / |\log \kappa_j| \to \infty \quad \text{as } j \to \infty, \tag{2.20}$$

where the integration is along the natural orientation given by $H_{\operatorname{Re} a_j p}$ on Γ_j starting at $w_j \in \mathring{\Gamma}_j$. (Actually, it suffices that the minimum in (2.20) is sufficiently large, depending on the norms of the symbol of the operator.) Since $|H_p| \ge \kappa_j \to 0$ on Γ_j, we find that condition (2.20) is well defined independently of the choice of multiplier a_j satisfying (2.18).

Observe that if (2.20) holds then there must be a change of sign of $\operatorname{Im} a_j p_s$ from $-$ to $+$ on Γ_j, and

$$\max_{\Gamma_j} (-1)^{\pm 1} \operatorname{Im} a_j p_s / |H_p| |\log \kappa_j| \to \infty \qquad j \to \infty \tag{2.21}$$

for both signs. Observe that condition (2.20) for a_j satisfying (2.18) is invariant under symplectic changes of coordinates and multiplication with elliptic pseudodifferential operators, thus under conjugation with elliptic Fourier integral operators. In fact, multiplication only changes the subprincipal symbol with uniform non-vanishing factors and terms proportional to $|\nabla p| = |H_p|$. By multiplying with a_j we may for simplicity assume that $a_j \equiv 1$. Then by choosing symplectic coordinates $(t, x; \tau, \xi)$ near a given point $w_0 \in \Gamma_j$ so that $\operatorname{Re} p = \alpha\tau$ near w_0 with $\alpha = |\operatorname{Re} \nabla p| \ne 0$, we obtain that $\partial_{x_k} \partial_{\xi_k} \operatorname{Re} p = 0$ at Γ_j, $\forall\ k$, and $\partial_t \partial_\tau \operatorname{Re} p = \partial_t \alpha = \partial_t |\operatorname{Re} \nabla p|$ at Γ_j near w_0. Thus, the second term in (2.19) only gives terms which are either real or gives terms in condition (2.20) which are bounded by

$$\left|\int \partial_t |\operatorname{Re}\nabla p|/|\nabla \operatorname{Re} p|\, ds/|\log(\kappa_j)|\right| = \mathcal{O}(|\log(|\nabla \operatorname{Re} p|)|/|\log(\kappa_j)|) = \mathcal{O}(1) \tag{2.22}$$

when $j \gg 1$ since $|\operatorname{Re}\nabla p| \cong |\nabla p| \geq \kappa_j \to 0$ on Γ_j by (2.18). Thus we obtain the following result.

Remark 2.8. We may replace the subprincipal symbol p_s by p_{m-1} in (2.20), since the difference is bounded as $j \to \infty$.

One can define the *reduced principal symbol* as $p + p_s$, see Definition 18.1.33 in [5]. Then (2.20) means that a non-homogeneous version of condition (Ψ) does not hold for the reduced principal symbol.

Example 2.9. If p is real and vanishes of exactly order $k \geq 2$ at an involutive manifold Σ_2, then we find that $|H_p| \cong d^{k-1}$ on S^*X where d is the homogeneous distance to Σ_2. If $\operatorname{Im} p_s$ changes sign from $-$ to $+$ on the semibicharacteristics and vanishes of order ℓ at Σ_2, then (2.20) holds if and only if $\ell < k-1$. When $k = 2$, this means that $\operatorname{Im} p_s$ changes sign from $-$ to $+$ on the limit bicharacteristic, as in the results of [6] and [7].

We shall study the microlocal solvability, which is given by the following definition. Recall that $H^{loc}_{(s)}(X)$ is the set of distributions that are locally in the L^2 Sobolev space $H_{(s)}(X)$.

Definition 2.10. *If $K \subset S^*X$ is a compact set, then we say that P is microlocally solvable at K if there exists an integer N so that for every $f \in H^{loc}_{(N)}(X)$ there exists $u \in \mathcal{D}'(X)$ such that $K \cap \operatorname{WF}(Pu - f) = \emptyset$.*

Observe that solvability at a compact set $M \subset X$ is equivalent to solvability at $S^*X\big|_M$ by [5, Theorem 26.4.2], and that solvability at a set implies solvability at a subset. Also, by Proposition 26.4.4 in [5] the microlocal solvability is invariant under conjugation by elliptic Fourier integral operators and multiplication by elliptic pseudodifferential operators. The following is the main result of the paper.

Theorem 2.11. *Let $P \in \Psi^m_{cl}(X)$ have principal symbol $\sigma(P) = p$ satisfying condition* (Ψ)*, and subprincipal symbol p_s. Let $\Gamma_j \subset S^*X$, $j = 1, \dots$ be a uniform family of semibicharacteristics of p so that* (2.8), (2.11), (2.13) *and* (2.20) *hold for some a_j satisfying* (2.18) *and grazing Lagrangean spaces L_j of Γ. Then P is not microlocally solvable at any limit semibicharacteristics of $\{\Gamma_j\}_j$.*

In fact, if there exists a limit semibicharacteristic, then we can choose a subsequence of semibicharacteristics Γ_j converging to it, which gives conditions (2.3) and (2.4) for these Γ_j, $\forall\, j$. Observe that if the principal symbol is real, then conditions (Ψ), (2.11) and (2.13) are trivially satified, and we obtain Theorem 2.9 in [2].

To prove Theorem 2.11 we shall use the following result. Let $\|u\|_{(k)}$ be the L^2 Sobolev norm of order k for $u \in C_0^\infty$ and P^* the L^2 adjoint of P.

Remark 2.12. If P is microlocally solvable at $\Gamma \subset S^*X$, then Lemma 26.4.5 in [5] gives that for any $Y \Subset X$ such that $\Gamma \subset S^*Y$ there exists an integer ν and a pseudodifferential operator A so that $\mathrm{WF}(A) \cap \Gamma = \emptyset$ and

$$\|u\|_{(-N)} \le C(\|P^*u\|_{(\nu)} + \|u\|_{(-N-n)} + \|Au\|_{(0)}) \qquad u \in C_0^\infty(Y) \tag{2.23}$$

where N is given by Definition 2.10.

We shall use Remark 2.12 to prove Theorem 2.11 in Section 6 by constructing approximate local solutions to $P^*u = 0$. We shall first prepare and get a microlocal normal form for the adjoint operator, which will be done in Section 3. We shall then apply P^* to an oscillatory solution, for which we shall solve the eikonal equation in Section 4 and the transport equations in Section 5.

3. The normal form

In the following we assume that the conditions in Theorem 2.11 holds with some limit semibicharacteristic, observe that then (2.3) and (2.4) hold for Γ_j. We shall prepare the operator to a normal form as in [2], but since the principal symbol now is complex valued the preparation will be slightly different. First we shall put the adjoint operator P^* on a normal form uniformly and microlocally near the semibicharacteristics $\Gamma_j \subset \Sigma \cap S^*X$ converging in C^∞ to $\Gamma \subset \Sigma_2$. This will present some difficulties since we only have conditions at the semibicharacteristics. By the invariance, we may multiply with an elliptic operator so that the order of P^* is $m = 1$ and P^* has the symbol expansion $p + p_0 + \cdots$, where p is the principal symbol. By Remark 2.8 we may assume that p_0 is the subprincipal symbol, and as before we shall assume (2.18) so that $|\operatorname{Re} \nabla p| \cong |\nabla p|$. Observe that $p = 0$ on Γ_j and for the adjoint the signs in (2.20) are reversed, changing it to

$$\max_{\partial \Gamma_j} \int \operatorname{Im} a_j p_0 |H_p|^{-1}\, ds / |\log \kappa_j| \to -\infty \quad \text{as } j \to \infty, \tag{3.1}$$

where κ_j given by (2.10). Changing the starting point w_j of the integration to the maximum of the integral in (3.1) only improves the estimate so we may assume that

$$\int \operatorname{Im} a_j p_0 / |H_p|\, ds \le 0 \quad \text{on } \Gamma_j \tag{3.2}$$

with equality at $w_j \in \Gamma_j$. Since ∇p_0 and ∇H_p are bounded on S^*X and $|H_p| \ge \kappa_j$ on Γ_j, we find that $|H_p|$ and $p_0/|H_p|$ only change with a fixed factor and a bounded term on an interval of length $\lesssim \kappa_j$ on Γ_j. Thus, we find that integrating $\operatorname{Im} a_j p_0 / |H_p|$ over such intervals only gives bounded terms. Therefore, by (2.21) we may assume that

$$|\Gamma_j| \gg \kappa_j \tag{3.3}$$

and that condition (3.1) holds on some intervals of length $\cong \kappa_j$ at the endpoints of Γ_j.

Now we choose

$$1 \le \lambda_j = \kappa_j^{-1/\varepsilon} \Longleftrightarrow \kappa_j = \lambda_j^{-\varepsilon} \tag{3.4}$$

for some $0 < \varepsilon \le 1$ to be determined later. Then we may replace $|\log \kappa_j|$ with $\log \lambda_j$ in (3.1). By choosing a subsequence and renumbering, we may assume by (2.20) that

$$\max_{\partial\Gamma_j} \int \operatorname{Im} a_j p_0/|H_p|\, ds \le -j \log \lambda_j \tag{3.5}$$

and that this also holds on some intervals of length $\cong \kappa_j$ at the endpoints of Γ_j. Next, we introduce the normalized principal and subprincipal symbols

$$\widetilde{p} = p/|H_p| \quad \text{and} \quad \widetilde{p}_0 = p_0/|H_p|. \tag{3.6}$$

Then we have that $H_{\widetilde{p}}\big|_{\Gamma_j} \in C^\infty$ uniformly for the grazing Lagrangean space L_j of Γ_j, $|H_{\widetilde{p}}| = 1$ on Γ_j and $dH_{\widetilde{p}}\big|_{L_j}$ is uniformly bounded at Γ_j by (2.4) and (2.7). We find that condition (3.5) becomes

$$\max_{\partial\Gamma_j} \int \operatorname{Im} a_j \widetilde{p}_0\, ds \le -j \log \lambda_j. \tag{3.7}$$

Observe that because of condition (2.21) we have that $\partial\Gamma_j$ has two components since $\operatorname{Im} a_j \widetilde{p}_0$ has opposite sign there, thus Γ_j is a uniformly embedded curve.

In the following we shall consider a fixed semibicharacteristic $\Gamma_j \subset \Sigma \cap S^*X$ and suppress the index j, so that $a = a_j$, $\Gamma = \Gamma_j$, $L = L_j$ and $\kappa = \lambda^{-\varepsilon} = \kappa_j$ for some $\varepsilon > 0$ to be determined later. Observe that the preparation will be uniform in j with λ as parameter, assuming the conditions in Theorem 2.11. Now $H_{\operatorname{Re} a\widetilde{p}} \in C^\infty$ uniformly on Γ but not in a neighborhood. By (2.4) we may define the first order Taylor expansion of $\operatorname{Re} a\widetilde{p}$ at Γ uniformly. Since $\Gamma \in C^\infty$ uniformly, we can choose local uniform coordinates so that $\Gamma = \{\, (t, 0)) : \ t \in I \subset \mathbf{R} \,\}$ locally. In fact, we can take a local parametrization $\gamma(t)$ of Γ with respect to the arc length and choose the orthogonal space $M \subset \mathbf{R}^{n-1}$ to the tangent vector of Γ at a point w_0 with respect to some local Riemannean metric. Then $\mathbf{R} \times M \ni (t, w) \mapsto \gamma(t) + w$ is uniformly bounded in C^∞ with a uniformly bounded inverse near $(t_0, 0)$ giving local coordinates near $\Gamma = \{\, (t, 0) : t \in I \,\}$. We may then complete t to a uniform symplectic coordinate system. Multiplying with the uniformly bounded function $a(t, 0)$ we may assume that $a(t, 0) \equiv 1$. We can define the first order Taylor term of $\operatorname{Re} \widetilde{p}$ at Γ by

$$\varrho(t, w) = \partial_w \operatorname{Re} \widetilde{p}(t, 0) \cdot w, \qquad w = (x, \tau, \xi), \tag{3.8}$$

which is uniformly bounded. This can be done locally, and by using a uniformly bounded partition of unity we obtain this in a fixed neighborhood of Γ. Going back to the original coordinates, we find that $\varrho \in C^\infty$ uniformly near Γ and $\operatorname{Re} \widetilde{p} - \varrho = \mathcal{O}(d^2)$, but the error is not uniformly bounded. Here d is the homogeneous distance to Γ, i.e., the distance with respect to the homogeneous metric

$$dt^2 + |dx|^2 + (d\tau^2 + |d\xi|^2)/\langle(\tau, \xi)\rangle^2. \tag{3.9}$$

But by condition (2.7) we find that the second order derivatives of $\widetilde{p}$ along the Lagrangean space L at Γ are uniformly bounded. We shall use homogeneous coordinates, i.e., local coordinates which are normalized with respect to the homogeneous metric (3.9).

By completing $\tau = \varrho$ in (3.8) to a uniformly bounded homogeneous symplectic coordinate system $(\tau, w) = (\tau, x, \tau, \xi)$ near Γ and conjugating with the corresponding uniformly bounded Fourier integral operator we may assume that

$$\Gamma = \{ (t, 0; 0, \xi_0) : \; t \in I \} \subset S^*\mathbf{R}^n \tag{3.10}$$

for $|\xi_0| = 1$ and some bounded interval $I \ni 0$, and that $\operatorname{Re} \widetilde{p} \cong \tau$ modulo second order terms at Γ. The second order terms are not uniformly bounded, but $d\nabla\widetilde{p}\big|_L$ is uniformly bounded at Γ by (2.7). Since $d \operatorname{Re} \widetilde{p} = d\tau$ on Γ we find that $H_{\operatorname{Re} \widetilde{p}}\big|_\Gamma = D_t$ and since $L \subset (dp)^{-1}(0)$ we may obtain that $L = \{ (t, x; 0, 0) \}$ at any given point at Γ by choosing suitable linear symplectic coordinates (x, ξ). We find from (2.7) that

$$\big| d\nabla\widetilde{p}(t, 0; 0, \xi_0)\big|_L \big| \lesssim 1, \quad t \in I. \tag{3.11}$$

Condition (2.15) gives

$$|\partial_{t,x,\xi} \operatorname{Im} \widetilde{p}(t, 0; 0, \xi_0)| \lesssim \kappa^{14/3} = \lambda^{-14\varepsilon/3}, \quad t \in I, \tag{3.12}$$

and condition (2.16) gives

$$\big| d\, \partial_{t,x,\xi} \operatorname{Im} \widetilde{p}(t, 0; 0, \xi_0)\big|_L \big| \lesssim \lambda^{-4\varepsilon/3}, \quad t \in I. \tag{3.13}$$

Here $a \lesssim b$ (and $b \gtrsim a$) means that $a \le Cb$ for some $C > 0$.

Let

$$q(t, w) = |\nabla p(t, w)| \ge \lambda^{-\varepsilon} \quad \text{at } \Gamma \tag{3.14}$$

and extend q so that it is homogeneous of degree 0, then q is the norm of the *homogeneous gradient* of p. Recall that $\lambda \gg 1$ is a parameter that depends on the bicharacteristic Γ. Since the symbols are homogeneous, we shall restrict them to $S^*\mathbf{R}^n$. There we shall choose coordinates (t, w) so that $w = 0$ on Γ, and then localize in conical neighborhoods depending on the parameter λ. We have $|\nabla\widetilde{p}| \equiv 1$ at Γ, higher derivatives are not uniformly bounded but can be handled by the using the metric

$$g_\varepsilon = (dt^2 + |dw|^2)\lambda^{2\varepsilon}, \quad w = (x, \tau, \xi), \tag{3.15}$$

and the symbol classes $f \in S(m, g_\varepsilon)$ defined by $\partial^\alpha f = \mathcal{O}(m\lambda^{|\alpha|\varepsilon})$, $\forall\, \alpha$.

Proposition 3.1. *If* (3.10) *and* (3.14) *hold then q is a weight for g_ε, $q \in S(q, g_\varepsilon)$ and $\widetilde{p}(t, w) \in S(\lambda^{-\varepsilon}, g_\varepsilon)$ when $|w| \le c\lambda^{-\varepsilon}$ for some $c > 0$ on $S^*\mathbf{R}^n$ when $t \in I$.*

This gives $p = q\widetilde{p} \in S(q\lambda^{-\varepsilon}, g_\varepsilon)$ when $|w| \le c\lambda^{-\varepsilon}$. Observe that $b \in S^{\mu}_{1-\varepsilon,\varepsilon}$ if and only if $b \in S(\lambda^\mu, g_\varepsilon)$ in homogeneous coordinates when $|\xi| \cong \lambda \gtrsim 1$. In fact, in homogeneous coordinates z this means that $\partial_z^\alpha b = \mathcal{O}(|\xi|^{\mu+|\alpha|\varepsilon})$. Therefore, we obtain by homogeneity that $\widetilde{p} \in S^{1-\varepsilon}_{1-\varepsilon,\varepsilon}$ and $q^{-1} \in S^{\varepsilon}_{1-\varepsilon,\varepsilon}$ when $|w| \lesssim \lambda^{-\varepsilon} \cong |\xi|^{-\varepsilon} \lesssim 1$.

Proof. We are going to use the previously chosen coordinates (t, w) on $S^*\mathbf{R}^n$ so that $\Gamma = \{ (t, 0) : t \in I \}$. Now $\partial^2 p = \mathcal{O}(1)$, $q \ge \lambda^{-\varepsilon}$ at Γ by (3.14) and

$$\partial q = \operatorname{Re} \nabla \overline{p} \cdot (\partial \nabla p)/q \quad \text{when } q \neq 0, \tag{3.16}$$

which is uniformly bounded. We find that $q(s, w) \cong q(t, 0)$ when $|s-t|+|w| \le c\lambda^{-\varepsilon}$ for small enough $c > 0$, so q is a weight for g_ε there. This gives that $|p(t, w)| \lesssim q(t, w)\lambda^{-\varepsilon}$, $|\nabla p(t, w)| = q(t, w)$ and $|\partial^\alpha p| \lesssim 1 \lesssim q\lambda^\varepsilon \lesssim q\lambda^{(|\alpha|-1)\varepsilon}$ for $|\alpha| \ge 2$, which gives $p \in S(q\lambda^{-\varepsilon}, g_\varepsilon)$ when $|w| \le c\lambda^{-\varepsilon}$ and $t \in I$.

We find from (3.16) that $\partial q = \alpha/q$ where $\alpha \in S(q^2\lambda^\varepsilon, g_\varepsilon)$ when $|w| \le c\lambda^{-\varepsilon}$ since $\nabla p \in S(q, g_\varepsilon)$ in this domain. By induction over the order of differentiation of q we obtain from (3.16) that $q \in S(q, g_\varepsilon)$ when $|w| \le c\lambda^{-\varepsilon}$, which gives the result. □

As before, we take the restriction of $\widetilde{p}$ to $|\xi| = 1$, use local coordinates (t, w) on $S^*\mathbf{R}^n$ so that (3.10) holds with $\xi_0 = 0$ and put $Q(t, w) = \lambda^\varepsilon \widetilde{p}(t\lambda^{-\varepsilon}, w\lambda^{-\varepsilon})$ when $t \in I_\varepsilon = \{ t\lambda^\varepsilon : t \in I \}$. Recall that $\lambda \gg 1$ is fixed, depending on Γ. Then by Proposition 3.1 we find that $Q \in C^\infty$ uniformly when $|w| \lesssim 1$ and $t \in I_\varepsilon$, $\partial_\tau \operatorname{Re} Q \equiv 1$ and $|\partial_{t,x,\xi} \operatorname{Re} Q| \equiv 0$ when $w = 0$ and $t \in I_\varepsilon$. Thus we find $|\partial_\tau Q| \neq 0$ for $|w| \lesssim 1$ and $t \in I_\varepsilon$. By using Taylor's formula at Γ we can write $Q(t, x; \tau, \xi) = \tau + h(t, x; \tau, \xi)$ when $|w| \lesssim 1$ and $t \in I_\varepsilon$, where $h = |\nabla \operatorname{Re} h| = 0$ at $w = 0$. By using the Malgrange preparation theorem, we obtain

$$\tau = a(t, w)(\tau + h(t, w)) + s(t, x, \xi), \quad |w| \lesssim 1, \ t \in I_\varepsilon,$$

where a and $s \in C^\infty$ uniformly, $a \neq 0$, and on Γ we have $a = 1$ and $s = |\nabla \operatorname{Re} s| = 0$. In fact, this can be done uniformly, first locally in t and then by a uniform partition of unity for $t \in I_\varepsilon$. This gives

$$a(t, w)Q(t, w) = \tau - s(t, x, \xi), \quad |w| \lesssim 1, \ t \in I_\varepsilon. \tag{3.17}$$

In the original coordinates, we find that

$$\lambda^\varepsilon \widetilde{p}(t, w) = a^{-1}(t\lambda^\varepsilon, w\lambda^\varepsilon)(\tau\lambda^\varepsilon - s(t\lambda^\varepsilon, x\lambda^\varepsilon, \xi\lambda^\varepsilon))$$

and thus

$$\widetilde{p}(t, w) = b(t, w)(\tau - r(t, x, \xi)), \qquad |w| \lesssim \lambda^{-\varepsilon}, \ t \in I, \tag{3.18}$$

where $0 \neq b \in S(1, g_\varepsilon)$, $r(t, x, \xi) = \lambda^{-\varepsilon} s(t\lambda^\varepsilon, x\lambda^\varepsilon, \xi\lambda^\varepsilon) \in S(\lambda^{-\varepsilon}, g_\varepsilon)$ when $|w| \lesssim \lambda^{-\varepsilon}$, and $t \in I$, $b = 1$ and $r = |\nabla \operatorname{Re} r| = 0$ on Γ. By condition (3.11) we find that

$$\big|d\nabla r\big|_L\big| \le C \quad \text{at } \Gamma \tag{3.19}$$

since r is constant in τ. Similarly, by conditions (3.12) and (3.13) we find that

$$|\nabla \operatorname{Im} r| \lesssim \lambda^{-14\varepsilon/3} \quad \text{at } \Gamma \tag{3.20}$$

and

$$\big|d\nabla \operatorname{Im} r\big|_L\big| \le C\lambda^{-4\varepsilon/3} \quad \text{at } \Gamma. \tag{3.21}$$

Extending by homogeneity, we obtain this preparation where the homogeneous distance in (x, ξ) to Γ is $\lesssim \lambda^{-\varepsilon}$, then (3.19)–(3.21) hold with the homogeneous gradient. Now, the symbol b is homogeneous but it is not in $S^0_{1,0}$ uniformly, instead it will have uniform bounds in a larger symbol class. In the following, we shall denote by Γ the rays in $T^*\mathbf{R}^n$ that goes through the semibicharacteristic. Recall that $\widetilde{p} = p/q$, where $q \in S(q, g_\varepsilon)$ when $|w| \lesssim \lambda^{-\varepsilon}$ and is homogeneous of degree 0. By homogeneity we obtain from (3.18) that

$$b^{-1}q^{-1}p(t,x;\tau,\xi) = \tau - r(t,x,\xi)$$

where $b^{-1} \in S^0_{1-\varepsilon,\varepsilon}$, $q^{-1} \in S^\varepsilon_{1-\varepsilon,\varepsilon}$ and $\tau - r \in S^{1-\varepsilon}_{1-\varepsilon,\varepsilon}$ when $|\xi| \gtrsim \lambda$ and the homogeneous distance $d(x,\xi)$ to $(0,\xi_0)$ is less than $c|\xi|^{-\varepsilon} \lesssim \lambda^{-\varepsilon}$, $c > 0$. In fact, in homogeneous coordinates this means that $b^{-1} \in S(1, g_\varepsilon)$, $q^{-1} \in S(\lambda^\varepsilon, g_\varepsilon)$ and $r \in S(\lambda^{1-\varepsilon}, g_\varepsilon)$ when $|\xi| \cong \lambda$.

Take a homogeneous cut-off function $\chi(x,\xi) \in S^0_{1,0}$ supported where $d(x,\xi) \lesssim \lambda^{-\varepsilon}$ so that $b \ge c_0 > 0$ in $\operatorname{supp}\chi$ and $\chi = 1$ when $d \le c\lambda^{-\varepsilon}$ for some $c > 0$, then we have $\chi \in S^0_{1-\varepsilon,\varepsilon}$ uniformly when $|\xi| \gtrsim \lambda$. We take the homogeneous symbol $B = \chi b^{-1}q^{-1} \in S^\varepsilon_{1-\varepsilon,\varepsilon}$ uniformly when $|\xi| \gtrsim \lambda$ and we compose the corresponding pseudodifferential operator $B \in \Psi^\varepsilon_{1-\varepsilon,\varepsilon}$ with P^*. Since $P^* \in \Psi^1_{1,0}$ we obtain an asymptotic expansion of BP^* in $S^{1+\varepsilon-j(1-\varepsilon)}_{1-\varepsilon,\varepsilon}$ for $j = 0, 1, 2, \dots$ when $|\xi| \gtrsim \lambda$. But actually the symbol is in a better class. The principal symbol is

$$(\tau - r(t,x,\xi))\chi \in S^{1-\varepsilon}_{1-\varepsilon,\varepsilon} \quad \text{for } |\xi| \gtrsim \lambda,$$

and the calculus gives that the homogeneous term is equal to

$$\frac{i}{2}H_p(\chi b^{-1}q^{-1}) + \chi b^{-1}q^{-1}p_0 \tag{3.22}$$

where p_0 is the homogeneous term of the expansion of P^*. As before, we shall use homogeneous coordinates. Then Proposition 3.1 gives $p = q\widetilde{p} \in S(q\lambda^{-\varepsilon}, g_\varepsilon)$ when $|\xi| \cong \lambda$ and since $\chi b^{-1}q^{-1} \in S(q^{-1}, g_\varepsilon) \subset S(\lambda^\varepsilon, g_\varepsilon)$ when $|\xi| \cong \lambda$, we find that the terms in (3.22) are in $S(\lambda^\varepsilon, g_\varepsilon)$ when $d \lesssim \lambda^{-\varepsilon}$ and by homogeneity in $S^\varepsilon_{1-\varepsilon,\varepsilon}$ when $d \lesssim |\xi|^{-\varepsilon} \lesssim \lambda^{-\varepsilon}$. The value of H_p at Γ is equal to $q\partial_t$ modulo terms with coefficients that are $\mathcal{O}(\lambda^{-14\varepsilon/3})$ by (3.20) so the value of (3.22) is equal to

$$\frac{1}{2i}\partial_t q/q + p_0/q = \frac{D_t|\nabla p|}{2|\nabla p|} + \frac{p_0}{|\nabla p|} \quad \text{at } \Gamma \tag{3.23}$$

modulo $\mathcal{O}(\lambda^{-8\varepsilon/3})$. Here $|\nabla p| = \sqrt{|\partial_x p|^2/|\xi|^2 + |\partial_\xi p|^2}$ is the homogeneous gradient, and the error of this approximation is bounded by $\lambda^{2\varepsilon}$ times the homogeneous distance d to Γ, since (3.22) is in $S(\lambda^\varepsilon, g_\varepsilon)$. Observe that $p_0/|\nabla p|$ is equal to the normalized subprincipal symbol of P^* on $S^*\mathbf{R}^n$ given by (3.6). But we have to estimate the error terms in this preparation.

Definition 3.2. *For $0 < \varepsilon < 1/2$ and $R \in S^\mu_{\varrho,\delta}$ where $\varrho + \delta \ge 1$, $\varrho > \varepsilon$ and $\delta < 1 - \varepsilon$, we say that $S^*X \ni (x_0,\xi_0) \notin \mathrm{WF}_\varepsilon(R)$ if for any N there exists $c_N > 0$ so that $R \in S^{-N}_{\varrho,\delta}$ when the homogeneous distance to the ray $\{\, (x_0, \varrho\,\xi_0) : \ \varrho \in \mathbf{R}_+ \,\}$ is less than $c_N|\xi|^{-\varepsilon}$.*

For a family of operators $R_j \in \Psi^\mu_{\varrho,\delta}$, $j = 1, \dots,$ we say that $S^*X \ni (x_j,\xi_j) \notin \mathrm{WF}_\varepsilon(R_j)$ uniformly with respect to $\lambda_j \ge 1$, if for any N there exists $C_N > 0$

so that $R_j \in S^{-N}_{\varrho,\delta}$ *uniformly in* j *when the homogeneous distance to the ray* $\{\,(x_j, \varrho\,\xi_j) :\ \varrho \in \mathbf{R}_+\,\}$ *is less than* $C_N|\xi|^{-\varepsilon} \le CC_N\lambda_j^{-\varepsilon}$ *for some* $C > 0$.

By the calculus, this means that there exist $A_j \in \Psi^0_{1-\varepsilon,\varepsilon}$ so that $A_j \ge c > 0$ when the distance to the ray through (x_j, ξ_j) is less than $C_N|\xi|^{-\varepsilon} \lesssim \lambda_j^{-\varepsilon}$ such that $A_jR_j \in \Psi^{-N}$ uniformly. This neighborhood is in fact the points with fixed g_ε distance to the ray through (x_j, ξ_j) when $|\xi| \gtrsim \lambda_j$. For example, if the homogeneous cut-off functions χ_j is equal to 1 where the homogeneous distance to the ray $\{\,(x_j, \varrho\,\xi_j) :\ \varrho \in \mathbf{R}_+\,\}$ is less than $C_N\lambda_j^{-\varepsilon}$ then $(x_j, \xi_j) \notin \mathrm{WF}_\varepsilon(1-\chi_j)$ uniformly with respect to λ_j. It follows from the calculus that Definition 3.2 is invariant under composition with classical elliptic pseudodifferential operators and under conjugation with elliptic homogeneous Fourier integral operators preserving the fiber, by the conditions on ϱ and δ. We also have that $\mathrm{WF}_\varepsilon(R)$ grows when ε shrinks and $\mathrm{WF}_\varepsilon(R) \subset \mathrm{WF}(R)$.

Now we can use the Malgrange division theorem in order to make the lower order terms independent on τ when $d \lesssim \lambda^{-\varepsilon}$, starting with the subprincipal symbol $\widetilde{p}_0 \in S^\varepsilon_{1-\varepsilon,\varepsilon}$ of BP^* given by (3.22). Then restricting to $|\xi| = 1$ and rescaling as before so that $Q_0(t,w) = \lambda^{-\varepsilon}\widetilde{p}_0(t\lambda^{-\varepsilon}, w\lambda^{-\varepsilon}) \in C^\infty$ uniformly, we obtain that

$$Q_0(t,w) = \widetilde{c}(t,w)(\tau - s(t,x,\xi)) + \widetilde{q}_0(t,x,\xi), \quad |w| \lesssim 1,\ t \in I_\varepsilon,$$

where s is given by (3.17), and $\widetilde{c}$ and $\widetilde{q}_0$ are uniformly in C^∞. This can be done uniformly, first locally and then by a partition of unity for $t \in I_\varepsilon$. We find in the original coordinates that

$$\widetilde{p}_0(t,w) = c(t,w)(\tau - r(t,x,\xi)) + q_0(t,x,\xi), \quad d \lesssim \lambda^{-\varepsilon},\ t \in I, \tag{3.24}$$

where

$$q_0(t,w) = \lambda^\varepsilon\widetilde{q}_0(t\lambda^\varepsilon, w\lambda^\varepsilon) \in S(\lambda^\varepsilon, g_\varepsilon) \ \text{ and } \ c(t,w) = \lambda^{2\varepsilon}\widetilde{c}(t\lambda^\varepsilon, w\lambda^\varepsilon) \in S(\lambda^{2\varepsilon}, g_\varepsilon).$$

By using a partition of unity, we obtain (3.24) uniformly when the homogeneous distance to Γ is $\lesssim \lambda^{-\varepsilon}$. By homogeneity we find as before that c is homogeneous of degree -1 and q_0 is homogeneous of degree 0, which gives $c \in S^{2\varepsilon-1}_{1-\varepsilon,\varepsilon}$ and $q_0 \in S^\varepsilon_{1-\varepsilon,\varepsilon}$ when $|\xi| \gtrsim \lambda$. Now the composition of the operators having symbols c and $\tau - r$ gives error terms that are homogeneous of degree -1 and are uniformly in $S^{3\varepsilon-1}_{1-\varepsilon,\varepsilon}$ when $|\xi| \gtrsim \lambda$. Thus if $\varepsilon < 1/3$ then by multiplication with an pseudodifferential operator with symbol $1 - c$ we can make the subprincipal symbol independent of τ. By iterating this procedure we can successively make any lower order terms independent of τ when the homogeneous distance d to Γ is less than $c\lambda^{-\varepsilon}$. By applying a homogeneous cut-off function χ as before we obtain the following result.

Proposition 3.3. *Assume that* (2.3), (2.4), (2.8), (2.11), (2.13), *and* (2.20) *hold uniformly for* Γ_j, L_j *and* λ_j *satisfying* (3.4) *for some* $\varepsilon > 0$. *By conjugating with uniformly bounded elliptic homogeneous Fourier integral operators and multiplying with uniformly bounded homogeneous elliptic operators we may assume that* $m = 1$, $a_j \equiv 1$ *and* Γ_j *is given by* (3.10). *If* $0 < \varepsilon < 1/3$ *then for any* $c > 0$ *we can obtain* *that* $B_jP^* = Q_j + R_j \in \Psi^{1-\varepsilon}_{1-\varepsilon,\varepsilon}$ *where* $B_j \in \Psi^{\varepsilon}_{1-\varepsilon,\varepsilon}$ *uniformly,* $\Gamma_j \cap \mathrm{WF}_\varepsilon(R_j) = \emptyset$ *uniformly, and the symbol of* Q_j *is equal to*

$$\tau - r(t,x,\xi) + q_0(t,x,\xi) + r_0(t,x,\xi) \quad \text{when } d_j(x,\xi) \le c|\xi|^{-\varepsilon} \lesssim \lambda_j^{-\varepsilon} \text{ and } t \in I, \tag{3.25}$$

where d_j *is the homogeneous distance to* Γ_j*. Here* r *is homogeneous of degree 1 and* q_0 *is homogenous of degree 0,* $r \in S^{1-\varepsilon}_{1-\varepsilon,\varepsilon}$*,* $q_0 \in S^{\varepsilon}_{1-\varepsilon,\varepsilon}$ *and* $r_0 \in S^{3\varepsilon-1}_{1-\varepsilon,\varepsilon}$ *uniformly. We also have* $r = |\nabla \operatorname{Re} r| = 0$*,* $\nabla \operatorname{Im} r = \mathcal{O}\big(\lambda_j^{-14\varepsilon/3}\big)$*,* $d\nabla \operatorname{Re} r\big|_L = \mathcal{O}(1)$ *and* $d\nabla \operatorname{Im} r\big|_L = \mathcal{O}\big(\lambda_j^{-4\varepsilon/3}\big)$ *on* Γ_j*. We find that* q_0 *is equal to*

$$\frac{D_t|\nabla p(t,0)|}{2|\nabla p(t,0)|} + \frac{p_0(t,0)}{|\nabla p(t,0)|} \quad \text{when } d_j(x,\xi) \le c|\xi|^{-\varepsilon} \lesssim \lambda_j^{-\varepsilon} \text{ and } t \in I, \tag{3.26}$$

modulo terms that are $\mathcal{O}\big(\lambda^{-8\varepsilon/3} + \lambda^{2\varepsilon} d_j\big)$ *where* $|\nabla p| = \sqrt{|\partial_x p|^2/|\xi|^2 + |\partial_\xi p|^2}$ *is the homogeneous gradient of* p*.*

We shall apply the operator in Proposition 3.3 on oscillatory solutions having frequencies ξ of size λ, see Proposition 3.5. Observe also that the integration of the term $D_t|\nabla p(t,0)|/2|\nabla p(t,0)|$ in (3.26) will give terms that are

$$\mathcal{O}(\log(|\nabla p(t,0)|)) = \mathcal{O}(|\log(\lambda)| + 1)$$

which do not affect condition (2.20).

Recall that L is a smooth section of Lagrangean spaces $L(w) \subset T_w\Sigma \subset T_w(T^*\mathbf{R}^n)$, $w \in \Gamma$, such that the linearization of the Hamilton vector field $H_{\operatorname{Re} p}$ is in TL at Γ. Here $\Sigma = (\operatorname{Re} p)^{-1}(0)$ and $T_w\Sigma = \operatorname{Ker} d\operatorname{Re} p(w)$ where $d\operatorname{Re} p(w) \ne 0$ for $w \in \Gamma$. By Proposition 3.3 we may assume that $\Gamma = \{\,(t,0;0,\xi_0) :\ t \in I\,\}$, $0 \in I$, and we may parametrize $L(t) = L(w)$ where $w = (t,0,\xi_0)$ for $t \in I$. Now since $T^*\mathbf{R}^n$ is a linear space, we may identify the fiber of $T_w(T^*\mathbf{R}^n)$ with $T^*\mathbf{R}^n$. Since $L(w) \subset T_w\Sigma$ and $w \in \Gamma$ we find that $d\tau = 0$ in $L(w)$. Since $L(w)$ is Lagrangean, we find that t lines are parallel to $L(w)$. By choosing linear symplectic coordinates in (x,ξ) we obtain that $L(0) = \{\,(s,y;0,0) :\ (s,y) \in \mathbf{R}^n\,\}$, then by condition (3.19) we find that $\partial_x \nabla r(0,0,\xi_0)$ is uniformly bounded. Since $d\tau = 0$ on $L(t)$ and $L(t)$ is Lagrangean we find by continuity for small t that

$$L(t) = \{\,(s,y;0,A(t)y) :\ (s,y) \in \mathbf{R}^n\,\} \tag{3.27}$$

where $A(t)$ is real, continuous and symmetric for $t \in I$ and $A(0) = 0$. Since the linearization of the Hamilton vector field $H_{\operatorname{Re} p}$ at Γ is tangent to L, we find that L is parallel under the flow of that linearization. Since $L(t)$ is Lagrangean, the evolution of $t \mapsto L(t)$ is determined by the restriction of the second order Taylor expansion of $r(t,w)$ to $L(t)$. For (3.27) this restriction is given by the second order Taylor expansion of

$$R(t,x) = \operatorname{Re} r(t,x,\xi_0 + A(t)x)$$

thus $\partial_x^2 R(t,0)$ is uniformly bounded by condition (2.7). The linearized Hamilton vector field is

$$\partial_t + \langle \partial_x^2 R(t,0)x, \partial_\xi \rangle = \partial_t + \langle \big(\partial_x^2 \operatorname{Re} r(t,0,\xi_0) + \partial_x\partial_\xi \operatorname{Re} r(t,0,\xi_0)A \\ + A\partial_\xi\partial_x \operatorname{Re} r(t,0,\xi_0) + A\partial_\xi^2 \operatorname{Re} r(t,0,\xi_0)A\big)x, \partial_\xi\rangle.$$

Applying this on $\xi - A(t)x$, which vanishes identically on $L(t)$ for $t \in I$, we obtain that the evolution of $L(t)$ is given by

$$A'(t) = \partial_x^2 \operatorname{Re} r(t,0,\xi_0) + \partial_x\partial_\xi \operatorname{Re} r(t,0,\xi_0)A(t) \\ + A(t)\partial_\xi\partial_x \operatorname{Re} r(t,0,\xi_0) + A(t)\partial_\xi^2 \operatorname{Re} r(t,0,\xi_0)A(t) \tag{3.28}$$

with $A(0) = 0$. This is locally uniquely solvable and the right-hand side is uniformly bounded as long as A is bounded. Observe that by uniqueness, $A(t) \equiv 0$ if and only if $\partial_x^2 \operatorname{Re} r(t,0,\xi_0) \equiv 0$, $\forall\, t$. But since (3.28) is non-linear, the solution could become unbounded if $\partial_x^2 \operatorname{Re} r \neq 0$ and $\partial_\xi^2 \operatorname{Re} r \neq 0$ so that $\|A(s)\| \to \infty$ as $s \to t_1 \in I$. This means that the angle between $L(t) = \{\, (s,y;0,A(t)y) :\ (s,y) \in \mathbf{R}^n \,\}$ and the vertical space $\{\, (s,0;0,\eta) : (s,\eta) \in \mathbf{R}^n \,\}$ goes to zero, but that is only a coordinate singularity.

In general, since we identify the fiber of $T_w(T^*\mathbf{R}^n)$ with $T^*\mathbf{R}^n$ we may define $R(t,x,\xi)$ for each t so that

$$R(t,x,\xi) = \operatorname{Re} r(t,x,\xi_0+\xi) \quad \text{when } (0,x;0,\xi) \in L(t). \tag{3.29}$$

Then $R = \operatorname{Re} r$ on L and we find that

$$\tau - \langle R(t)z, z\rangle/2 \in C^\infty \tag{3.30}$$

if $z = (x,\xi)$ and $R(t) = \partial_z^2 R(t,0,0)\big|_L(t)$. Observe that we find from (3.19) that (3.30) is uniformly in C^∞ in z and uniformly continuous in t. We find that $R(0) = \partial_x^2 \operatorname{Re} r(t,0,\xi_0)$ and in general $R(t)$ is given by the right hand side of (3.28). Now we can complete t, $\tau - \langle R(t)z,z\rangle/2$ and $(x,\xi)\big|_{t=0}$ to a uniform homogeneous symplectic coordinates system so that $\Gamma = \{\, (t,0,\xi_0) :\ t \in I \,\}$ and $L(0) = \{\, (s,y;0,0) :\ (s,y) \in \mathbf{R}^n \,\}$. In fact, (x,ξ) satisfies a linear evolution equation $H_\tau(x,\xi) = 0$ and has the same value when $t = 0$, so $(x,\xi) = 0$ and $H_\tau = \partial_t$ on Γ. Since this is done by integration in t, it gives a uniformly bounded linear symplectic transformation in (x,ξ) which is uniformly C^1 in t. It is given by a uniformly bounded elliptic Fourier integral operator $F(t)$ on $\mathbf{R}^{n-1}$ which is uniformly C^1 in t. We will call this type of Fourier integral operator a *C^1-section of Fourier integral operators on $\mathbf{R}^{n-1}$*. This will give uniformly bounded terms when we conjugate $F(t)$ with a first order differential operator in t, for example the normal form of P^* given by (3.25). For t close to 0 the section $F(t)$ is given by multiplication with $e^{i\langle A(t)x,x\rangle}$, where $A(t)$ solves (3.28). For general t we can put $F(t)$ on this form after a linear symplectic transformation in (x,ξ). Observe that $F(t)$ is continuous on local L^2 Sobolev spaces in x, uniformly in t, since it is continuous with respect to the norm $\|(1+|x|^2+|D_x|^2)^k u\|$, $\forall\, k$. In fact, it suffices to check this for the generators of the group of Fourier integral operators corresponding to linear symplectic transformations of (x,ξ), which are given by the partial Fourier transforms, linear transformations in x and multiplication with $e^{i\langle Ax,x\rangle}$ where A is real and symmetric.

We find in the new coordinates that $p = \tau - r_1$, where $r_1(t,x,\xi)$ is independent of τ and satisfies $\partial_z^2 \operatorname{Re} r_1(t,0,0)\big|_L(t) \equiv 0$. This follows since

$$p(t,x;\tau,\xi) = \tau - \langle R(t)z,z\rangle/2 - r_1(t,x,\tau,\xi), \quad z = (x,\xi),$$

where $\partial_z^2 \operatorname{Re} r_1(t,0,0)\big|_L(t) \equiv 0$. We also have that $\partial_\tau r_1 = -\{\, t, r_1 \,\} = -\{\, t, r \,\} \equiv 0$, which is invariant under the change of symplectic coordinates. Similarly we find that the lower order terms $p_j(t,x,\xi)$ remain independent of τ for $j \le 0$. Since the evolution of L is determined by the second order derivatives of the principal symbol along L by Example 2.4, we find that $L(t) \equiv \{\, (t,x;0,0) : \ (t,x) \in \mathbf{R}^n \,\}$ after the change of coordinates. Since L is a grazing Lagrangean space, the linearization of $H_{\operatorname{Re} p}$ at Γ is tangent to L. Thus $\partial_x \operatorname{Re} r_1 = \partial_x^2 \operatorname{Re} r_1 = 0$, $\nabla \operatorname{Im} r_1 = \mathcal{O}\big(\lambda_j^{-14\varepsilon/3}\big)$ and condition (3.21) gives that $\partial_{t,x} \nabla \operatorname{Im} r_1 = \mathcal{O}\big(\lambda_j^{-4\varepsilon/3}\big)$ at Γ_j. Changing notation so that $r = r_1$ and $p(t,x;\tau,\xi) = \tau - r(t,x,\xi)$ we obtain the following result.

Proposition 3.4. *By conjugating with a uniformly bounded C^1 section of Fourier integral operators on $\mathbf{R}^{n-1}$, we may assume that the symplectic coordinates in Proposition* 3.3 *are chosen so that the grazing Lagrangean space*

$$L(w) \equiv \{\, (t,x,0,0) : \ (t,x) \in \mathbf{R}^n \,\}, \quad \forall\, w \in \Gamma,$$

which gives that $\partial_x \operatorname{Re} r = \partial_x^2 \operatorname{Re} r = 0$, $\partial_{t,x} \nabla \operatorname{Re} r = \mathcal{O}(1)$, $\nabla \operatorname{Im} r_1 = \mathcal{O}\big(\lambda_j^{-14\varepsilon/3}\big)$ and $\partial_{t,x} \nabla \operatorname{Im} r = \mathcal{O}\big(\lambda_j^{-4\varepsilon/3}\big)$ at Γ_j.

We shall apply the adjoint P^* of the operator on the form in Proposition 3.3 on approximate solutions on the form

$$u_\lambda(t,x) = \exp(i\lambda(\langle x,\xi_0\rangle + \omega(t,x))) \sum_{j=0}^{M} \varphi_j(t,x)\lambda^{-j\varrho} \tag{3.31}$$

where $|\xi_0| = 1$, the phase function $\omega(t,x) \in S(\lambda^{-7\varepsilon}, g_{3\varepsilon})$ is real valued and the amplitudes $\varphi_j(t,x) \in S(1, g_\delta)$ have support where $|x| \lesssim \lambda^{-\delta}$. Here $\delta \ge \varepsilon$ and ϱ are positive constants to be determined later. The phase function $\omega(t,x)$ will be constructed in Section 4, see Proposition 4.2. Observe that we have assumed that $\varepsilon < 1/3$ in Proposition 3.3, but we shall impose further restrictions on ε later on. We shall assume that $\varepsilon + \delta < 1$, then if $p(t,x,\xi) \in S^{1-\varepsilon}_{1-\varepsilon,\varepsilon}$ when $|\xi| \cong \lambda$ we obtain the asymptotic expansion

$$\begin{aligned} &p(t,x,D_x)(\exp(i\lambda(\langle x,\xi_0\rangle + \omega(t,x)))\varphi(t,x)) \\ &\sim \exp(i\lambda(\langle x,\xi_0\rangle + \omega(t,x))) \sum_\alpha \partial_\xi^\alpha p(t,x,\lambda(\xi_0 + \partial_x\omega(t,x)))\mathcal{R}_\alpha(\omega,\lambda,D)\varphi(t,x)/\alpha! \end{aligned} \tag{3.32}$$

where $\mathcal{R}_\alpha(\omega,\lambda,D)\varphi(t,x) = D_y^\alpha(\exp(i\lambda\widetilde{\omega}(t,x,y))\varphi(t,y))\big|_{y=x}$ with

$$\widetilde{\omega}(t,x,y) = \omega(t,y) - \omega(t,x) + (x-y)\partial_x\omega(t,x)$$

and the error term is of the same size as the next term in the expansion. See for example Theorem 3.1 in [8, Chap. VI], which is for classical pseudodifferential operators, phase functions and amplitudes, but the proof is easily adapted to the case when these depend uniformly on parameters. Observe that since $|\partial_x\omega| \cong \lambda^{-4\varepsilon} \ll 1$ the expansion only involves the values of $p(t,x,\xi)$ where $|\xi| \cong \lambda \gg 1$. Using this expansion we find that if p is given by (3.25) then

$$\begin{aligned} &e^{-i\lambda(\langle x,\xi_0\rangle+\omega(t,x))}p(t,x,D_{t,x})e^{i\lambda(\langle x,\xi_0\rangle+\omega(t,x))}\varphi(t,x) \\ &\quad\sim \lambda\big(\partial_t\omega(t,x) - r(t,x,\xi_0+\partial_x\omega)\big)\varphi(t,x) \\ &\qquad + D_t\varphi(t,x) - \sum_j \partial_{\xi_j} r(t,x,\xi_0+\partial_x\omega)D_{x_j}\varphi(t,x) + q_0(t,x,\xi_0+\partial_x\omega)\varphi(t,x) \\ &\qquad + \sum_{jk}\partial_{\xi_j}\partial_{\xi_k} r(t,x,\xi_0+\partial_x\omega)(\lambda^{-1}D_{x_j}D_{x_k}\varphi(t,x) + i\varphi(t,x)D_{x_j}D_{x_k}\omega(t,x))/2 \\ &\qquad + \cdots, \end{aligned} \tag{3.33}$$

which gives an expansion in $S(\lambda^{1-\varepsilon-j(1-\delta-\varepsilon)}, g_\delta)$, $j \ge 0$, if $\delta+\varepsilon<1$ and $\varepsilon < 1/4$. In fact, since $|\xi| \cong \lambda$ every ξ derivative on terms in $S^{1-\varepsilon}_{1-\varepsilon,\varepsilon}$ gives a factor that is $\mathcal{O}(\lambda^{\varepsilon-1})$ and every x derivative of φ gives a factor that is $\mathcal{O}(\lambda^{\delta})$. A factor $\lambda D_x^\alpha\omega$ requires $|\alpha| \ge 2$ number of ξ derivatives of a term in the expansion of P^*, which gives a factor that is $\mathcal{O}(\lambda^{1+(-7+3|\alpha|)\varepsilon-|\alpha|(1-\varepsilon)}) = \mathcal{O}(\lambda^{1-7\varepsilon-|\alpha|(1-4\varepsilon)}) = \mathcal{O}(\lambda^{-1+\varepsilon})$. Similarly, the expansion coming from terms in P^* that have symbols in $S^{\varepsilon}_{1-\varepsilon,\varepsilon}$ gives an expansion in $S^{\varepsilon-j(1-\delta-\varepsilon)}_{1-\varepsilon,\varepsilon}$, $j \ge 0$. Thus, if $\delta+\varepsilon < 2/3$ and $\varepsilon < 1/4$ then the terms in the expansion are $\mathcal{O}(\lambda^{\delta+2\varepsilon-1})$ except the terms in (3.33), and for the last ones we find that

$$\sum_{jk}\partial_{\xi_j}\partial_{\xi_k} r(t,x,\xi_0+\partial_x\omega)(\lambda^{-1}D_{x_j}D_{x_k}\varphi + i\varphi D_{x_j}D_{x_k}\omega) = \mathcal{O}(\lambda^{2\delta+\varepsilon-1} + \lambda^{3\varepsilon-\delta}). \tag{3.34}$$

In fact, $\partial_{\xi_j}\partial_{\xi_k} r(t,x,\xi_0+\partial_x\omega) = \mathcal{O}(\lambda^{\varepsilon})$ and $D_{x_j}D_{x_k}\omega = \mathcal{O}(\lambda^{2\varepsilon}d)$ when $\varphi \ne 0$, since we have $D_{x_j}D_{x_k}\omega = 0$ when $x=0$, and $d = \mathcal{O}(\lambda^{-\delta})$ in $\operatorname{supp}\varphi$.

The error terms in (3.34) are of equal size if $2\delta+\varepsilon-1 = 3\varepsilon-\delta$, thus $\delta = (1+2\varepsilon)/3 \ge \varepsilon$ since $\varepsilon \le 1$. Since $\delta+\varepsilon<1$ we obtain that $4\varepsilon-1 < 3\varepsilon-\delta = (7\varepsilon-1)/3 < 0$ if $\varepsilon < 1/7$ and $1-\delta-\varepsilon = (2-5\varepsilon)/3 > 1/3$ if $\varepsilon < 1/5$. Thus we obtain the following result.

Proposition 3.5. *Assume that p is given by (3.25), $\omega(t,x) \in S(\lambda^{-7\varepsilon}, g_{3\varepsilon})$ is real valued with $\partial_x\omega(t,0) \equiv \partial_x^2\omega(t,0) \equiv 0$, and $\varphi_j(t,x) \in S(1,g_\delta)$ has support where $|x| \lesssim \lambda^{-\delta}$ with positive δ and ε. If $\delta = (1+2\varepsilon)/3$ and $\varepsilon < 1/7$, then (3.33) has an expansion in $S(\lambda^{1-\varepsilon-j(2-5\varepsilon)/3}, g_\delta)$, $j \ge 0$, and is equal to*

$$\begin{aligned} &\lambda\big(\partial_t\omega(t,x) - r(t,x,\xi_0+\partial_x\omega)\big)\varphi(t,x) + D_t\varphi(t,x) \\ &\qquad - \sum_j \partial_{\xi_j} r(t,x,\xi_0+\partial_x\omega)D_{x_j}\varphi(t,x) + q_0(t,x,\xi_0+\partial_x\omega)\varphi(t,x) \end{aligned} \tag{3.35}$$

modulo terms that are $\mathcal{O}(\lambda^{(7\varepsilon-1)/3}) = \mathcal{O}(\lambda^{2\delta+\varepsilon-1})$.

In Sect. 5 we shall choose $\varepsilon = 1/8$ which gives $\delta = 5/12$, $(2-5\varepsilon)/3 = 11/24$ and $(7\varepsilon - 1)/3 = -1/24$, so we may take $\varrho = 1/24$ in (3.31).

4. The eikonal equation

Making the real part of the first term in the expansion (3.33) equal to zero gives the eikonal equation

$$\partial_t \omega - \operatorname{Re} s(t, x, \partial_x \omega) = 0, \qquad \omega(0, x) \equiv 0, \tag{4.1}$$

where $s(t, x, \xi) = r(t, x, \xi_0 + \xi)$. The imaginary part of the first term will be treated as a perturbation. We shall solve the eikonal equation approximatively after scaling, since we solve the real part it will be similar to the argument in [2]. We choose coordinates (t, x, ξ) on $S^*\mathbf{R}^n$ so that Γ is given by (3.10). We find that $s \in S(\lambda^{-\varepsilon}, g_\varepsilon)$ when $|x| + |\xi| \lesssim \lambda^{-\varepsilon}$ by Proposition 3.3, and we may assume that $L(t) \equiv \{\, (t, x, 0, 0) \,\}$, $\forall\, t$, by Proposition 3.4. But s is also in another symbol class by the following refinement of Proposition 3.3.

Proposition 4.1. *Assuming Propositions* 3.3 *and* 3.4 *we have*

$$s \in S(\lambda^{-7\varepsilon}, \lambda^{6\varepsilon}(dt^2 + |dx|^2) + \lambda^{8\varepsilon}|d\xi|^2)$$

when $|x| \lesssim \lambda^{-3\varepsilon}$, $|\xi| \lesssim \lambda^{-4\varepsilon}$ *and* $t \in I$.

Proof. Since $s \in S(\lambda^{-\varepsilon}, g_\varepsilon)$ when $|x| + |\xi| \lesssim \lambda^{-\varepsilon}$ by Proposition 3.3, we find that

$$|\partial_{t,x}^\alpha \partial_\xi^\beta s| \lesssim \lambda^{(|\alpha|+|\beta|-1)\varepsilon} \lesssim \lambda^{(3|\alpha|+4|\beta|-7)\varepsilon} \tag{4.2}$$

when $|x| + |\xi| \lesssim \lambda^{-\varepsilon}$, if and only $|\alpha| + |\beta| - 1 \le 3|\alpha| + 4|\beta| - 7$, i.e.,

$$2|\alpha| + 3|\beta| > 5.$$

Thus, we only have to check the cases $|\alpha|+|\beta| \le 2$ and $|\beta| \le 1$. Since the Lagrange remainder term is in the symbol class, we only have to check the derivatives at $x = \xi = 0$. Then we obtain (4.2) since $s(t, 0, 0) = 0$, $\partial s(t, 0, 0) = \mathcal{O}(\lambda^{-14\varepsilon/3})$ by (3.20), $\partial_{t,x}\partial_\xi s(t, 0, \xi_0) = \mathcal{O}(1)$ and $\partial_{t,x}^2 s(t, 0, 0) = \mathcal{O}(\lambda^{-4\varepsilon/3})$ by (3.19) and (3.21). □

Observe that the estimates for $\partial \operatorname{Im} s$ and $\partial_{t,x}\partial \operatorname{Im} s$ at Γ are better than the symbol estimates, which will be important in the proof of Lemma 5.2. Next, we scale and put $(x, \xi) = (\lambda^{-3\varepsilon} y, \lambda^{-4\varepsilon}\eta)$. When $|y| + |\eta| \le c$ we find

$$(y, \eta) \mapsto f(t, y, \eta) = \lambda^{7\varepsilon} s(t, \lambda^{-3\varepsilon} y, \lambda^{-4\varepsilon}\eta) \in C^\infty \tag{4.3}$$

and $y \mapsto \omega_0(t, y) = \lambda^{7\varepsilon}\omega(t, \lambda^{-3\varepsilon} y) \in C^\infty$ uniformly. Then the eikonal equation (4.1) is

$$\partial_t \omega_0 - \operatorname{Re} f(t, y, \partial_y \omega_0) \equiv 0, \qquad \omega_0(0, y) = 0, \tag{4.4}$$

when $|y| \le c$. We can solve (4.4) by solving the Hamilton–Jacobi equations:

$$\begin{cases} \partial_t y = -\partial_\eta \operatorname{Re} f(t, y, \eta), \\ \partial_t \eta = \partial_y \operatorname{Re} f(t, y, \eta), \end{cases} \tag{4.5}$$

with initial values $(y(0), \eta(0)) = (z, 0)$. Since we have uniform bounds on $(y, \eta) \mapsto f(t, y, \eta)$, we find that (4.5) has a uniformly bounded C^∞ solution $(y(t), \eta(t))$ if $(z, 0)$ is uniformly bounded. By taking z derivatives of the equations, we find that $z \mapsto (y(t, z), \eta(t, z)) \in C^\infty$ uniformly. By (4.5) we find that $(\partial_t y, \partial_t \eta)$ is uniformly bounded, and by taking repeated t, z derivatives of (4.5) we find that $\left(\partial_t^k \partial_z^\alpha y, \partial_t^k \partial_z^\alpha \eta\right) = \mathcal{O}(\lambda^{3(k-1)\varepsilon})$.

Letting $\partial_y \omega_0(t, y(t, z)) = \eta(t, z)$ and

$$\partial_t \omega_0(t, y(t, z)) = \operatorname{Re} f(t, y(t, z), \eta(t, z)) = \mathcal{O}(1)$$

when $|y| \le c$, we obtain the solution $\omega_0(t, y) \in S(1, \lambda^{6\varepsilon} dt^2 + |dy|^2)$ to (4.4). (Actually, we have $\partial_t \omega_0 \in S(1, \lambda^{6\varepsilon} dt^2 + |dy|^2)$.) Since $\nabla \operatorname{Re} f = 0$ on Γ we find by uniqueness that $y = \eta = 0$ when $z = 0$ which gives $\omega_0(t, 0) \equiv \partial_t \omega_0(t, 0) \equiv \partial_y \omega_0(t, 0) \equiv 0$. Since $\partial_{y,\eta} \operatorname{Re} f(t, 0, 0) = \partial_y^2 \operatorname{Re} f(t, 0, 0) = 0$ we find by differentiating (4.4) twice that

$$\begin{aligned}\partial_t \partial_y^2 \omega_0(t, 0) = \partial_y \partial_\eta \operatorname{Re} f(t, 0, 0) \partial_y^2 \omega_0(t, 0) + \partial_y^2 \omega_0(t, 0) \partial_\eta \partial_y \operatorname{Re} f(t, 0, 0) \\ + \partial_y^2 \omega_0(t, 0) \partial_\eta^2 \operatorname{Re} f(t, 0, 0) \partial_y^2 \omega_0(t, 0)\end{aligned}$$

Since $\partial_x^2 \omega(0, x) \equiv 0$ we find by uniqueness that $\partial_x^2 \omega(t, 0) \equiv 0$.

In the original coordinates we find that that if $x(0) = \mathcal{O}(\lambda^{-3\varepsilon})$ and $\xi(0) = 0$ then $x(t, x_0) = \mathcal{O}(\lambda^{-3\varepsilon})$ and $\xi(t, x_0) = \mathcal{O}(\lambda^{-4\varepsilon})$ for any $t \in I$. The scaling also gives that

$$\omega(t, x) = \lambda^{-7\varepsilon} \omega_0(t, \lambda^{3\varepsilon} x) \in S(\lambda^{-7\varepsilon}, g_{3\varepsilon}), \qquad |x| \lesssim \lambda^{-3\varepsilon}, \tag{4.6}$$

and we have $\omega(t, 0) \equiv \partial_x \omega(t, 0) \equiv \partial_x^2 \omega(t, 0) \equiv 0$. (Actually, $\partial_t \omega(t, x) \in S(\lambda^{-7\varepsilon}, g_{3\varepsilon})$ when $|x| \lesssim \lambda^{-3\varepsilon}$.) By the symbol estimates, we find $\partial \omega(t, x) = \mathcal{O}(\lambda^{-4\varepsilon})$ when $|x| \lesssim \lambda^{-3\varepsilon}$. Thus, we obtain the following result.

Proposition 4.2. *Let $0 < \varepsilon < 1/3$, and assume that Propositions 3.3 and 3.4 hold. Then there exists a real $\omega(t, x) \in S(\lambda^{-7\varepsilon}, g_{3\varepsilon})$ satisfying $\partial_t \omega = \operatorname{Re} r(t, x, \xi_0 + \partial_x \omega)$ when $|x| \lesssim \lambda^{-3\varepsilon}$ and $t \in I$ so that $\omega(t, 0) \equiv \partial_x \omega(t, 0) \equiv \partial_x^2 \omega(t, 0) \equiv 0$. If $3\varepsilon \le \delta \le 4\varepsilon$, we find that the values of $(t, x; \lambda \partial_t \omega(t, x), \lambda(\xi_0 + \partial_x \omega(t, x)))$ have homogeneous distance $\lesssim \lambda^{-\delta}$ to the rays through Γ when $|x| \lesssim \lambda^{-\delta}$ and $t \in I$.*

5. The transport equations

The next term in (3.33) is the transport equation, which by homogeneity is equal to

$$D_p \varphi + q_0 \varphi + i r_0 \varphi = 0 \quad \text{at } \Gamma = \{\, (t, 0; 0, \xi_0) : \ t \in I \,\} \tag{5.1}$$

where $D_p = D_t - \sum_j \partial_{\xi_j} r(t, x, \xi_0 + \partial_x \omega(t, x)) D_{x_j}$

$$r_0(t, x) = \lambda \operatorname{Im} r(t, x, \xi_0 + \partial_x \omega(t, x)) \tag{5.2}$$

and

$$q_0(t) \cong D_t |\nabla p(t, 0, \xi_0)| / 2 |\nabla p(t, 0, \xi_0)| + p_0(t, 0, \xi_0) / |\nabla p(t, 0, \xi_0)| = \mathcal{O}(\lambda^\varepsilon) \tag{5.3}$$

modulo $\mathcal{O}(\lambda^{-8\varepsilon/3}+\lambda^{2\varepsilon}|x|)$ when $|x| \lesssim \lambda^{-\varepsilon}$ by (3.26). Here the real valued $\omega(t,x) \in S(\lambda^{-7\varepsilon}, g_{3\varepsilon})$ is given by Proposition 4.2. Since the transport equation is given by a complex vector field, the treatment is different to the one in [2]. But essentially we shall treat the complex part of the transport equation as a perturbation.

Lemma 5.1. *If* $3\varepsilon \le \delta \le 7\varepsilon/2$ *then we have that*

$$D_p = D_t + \sum_j \langle a_j(t)\cdot x\rangle D_{x_j} + R(t,x,D)$$

where $a_j(t) \in C^\infty(\mathbf{R}, \mathbf{R}^{n-1})$ *uniformly* $\forall\, j$*, and* $R(t,x,D)$ *is a first-order differential operator in* x *with coefficients that are* $\mathcal{O}(\lambda^{3\varepsilon-2\delta})$ *when* $|x| \lesssim \lambda^{-\delta}$*.*

Proof. As before we shall use the translation $s(t,x,\xi) = r(t,x,\xi_0+\xi)$, then

$$s(t,x,\xi) \in S(\lambda^{-\varepsilon}, g_\varepsilon) \cap S(\lambda^{-7\varepsilon}, \lambda^{6\varepsilon}(dt^2+|dx|^2)+\lambda^{8\varepsilon}|d\xi|^2) \tag{5.4}$$

when $|x| \lesssim \lambda^{-3\varepsilon}$, $|\xi| \lesssim \lambda^{-4\varepsilon}$ and $t \in I$ by Proposition 4.2. Since $\partial_x^2\omega(t,0) \equiv 0$ we find from Taylor's formula that $a_j(t) = -\partial_x\partial_{\xi_j}\operatorname{Re} s(t,0,0)$ which is uniformly bounded by (3.19). The coefficients of the error term R are given by $\partial_\xi \operatorname{Im} s$ and the second order Lagrange remainder term of the coefficients of $\partial_\xi \operatorname{Re} s$. By Propositions 3.3, 3.4 and 4.2 we find from Taylor's formula that

$$\begin{aligned}\partial_\xi \operatorname{Im} s(t,x,\partial_x\omega(t,x)) &= \partial_\xi \operatorname{Im} s(t,0,0) + \partial_x\partial_\xi \operatorname{Im} s(t,0,0)x \\ &\qquad + \partial_\xi^2 \operatorname{Im} s(t,0,0)\partial_x\omega(t,x) + \mathcal{O}\big(\lambda^{2\varepsilon}(|x|^2+\lambda^{4\varepsilon}|x|^4)\big) \\ &= \mathcal{O}\big(\lambda^{-4\varepsilon}+\lambda^{-\varepsilon}|x|+\lambda^{3\varepsilon}|x|^2+\lambda^{-6\varepsilon}\big) = \mathcal{O}(\lambda^{3\varepsilon-2\delta})\end{aligned}$$

when $|x| \lesssim \lambda^{-\delta}$ since $3\varepsilon \le \delta \le 7\varepsilon/2$. In fact, $\partial_\xi \operatorname{Im} s = \mathcal{O}(\lambda^{-14\varepsilon/3})$ and $\partial_x\partial_\xi \operatorname{Im} s = \mathcal{O}(\lambda^{-4\varepsilon/3})$ at Γ, $\partial_\xi^2 s = \mathcal{O}(\lambda^{\varepsilon})$, $\partial^3 s = \mathcal{O}(\lambda^{2\varepsilon})$ and $\partial_x\omega(t,x) = \mathcal{O}(\lambda^{2\varepsilon}|x|^2) = \mathcal{O}(\lambda^{-4\varepsilon})$ when $|x| \lesssim \lambda^{-\delta}$ since $\delta \ge 3\varepsilon$. Similarly we find that the second order Lagrange remainder term of the coefficients of $\partial_\xi \operatorname{Re} s$ are $\mathcal{O}(\lambda^{2\varepsilon}(|x|^2+\lambda^{4\varepsilon}|x|^4)) = \mathcal{O}(\lambda^{2\varepsilon-2\delta})$ when $|x| \lesssim \lambda^{-\delta} \ll \lambda^{-\varepsilon}$, which proves the result. □

We also have to estimate the term $r_0(t,x) = \lambda \operatorname{Im} r(t,x,\partial_x\omega(t,x))$ which in fact is bounded according to the following lemma.

Lemma 5.2. *If* $\varepsilon = 1/8$ *and* $\delta = (1+2\varepsilon)/3 = 5/12$ *then* $r_0(t,x) \in S(1, g_\delta)$ *for* $|x| \lesssim \lambda^{-\delta}$ *and* $t \in I$*.*

Observe that we need that $\varepsilon < 1/7$ and $\delta = (1+2\varepsilon)/3$ in order to use the expansion of Proposition 3.5, and when $\varepsilon = 1/8$ we get $\delta = 5/12 = 10\varepsilon/3 < 7\varepsilon/2$.

Proof. As before we shall use scaling $(t,x,\xi) = (\lambda^{-3\varepsilon}s, \lambda^{-3\varepsilon}y, \lambda^{-4\varepsilon}\eta)$, and write $f(s,y,\eta) = \lambda^{7\varepsilon}r(t,x,\xi_0+\xi) \in C^\infty$ and $\omega_0(s,y) = \lambda^{7\varepsilon}\omega(t,x) \in C^\infty$ uniformly so that $\partial_y\omega_0(s,y) = \lambda^{4\varepsilon}\partial_x\omega(t,x)$ when $|x| \le c\lambda^{-3\varepsilon}$ and $t \in I$, which we shall assume in the following.

This gives

$$r_0(t,x) = \lambda^{1-7\varepsilon} \operatorname{Im} f(s,y,\partial_y\omega_0(t,y)), \tag{5.5}$$

and we shall show that

$$F(s,y) = \operatorname{Im} f(s,y,\partial_y\omega_0(t,y)) \in S(\lambda^{-\varepsilon}, g_\varrho) \quad \text{when } |y| \le c\lambda^{-\varrho},$$

where $\varrho = \delta - 3\varepsilon = \varepsilon/3$. Since $\varepsilon = 1/8$, this will give the result. Taylor's formula gives for $|y| \le c\lambda^{-\varrho}$,

$$\begin{aligned} F(s,y) = \partial_y \operatorname{Im} f(s,0,0)y + \langle \partial_y^2 \operatorname{Im} f(s,0,0)y,y\rangle/2 \\ + \partial_\eta \operatorname{Im} f(s,0,0)\langle\partial_y^3\omega_0(s,0)y,y\rangle/2 + R(s,y), \end{aligned} \tag{5.6}$$

where $R(s,y) \in C^\infty$ uniformly and is vanishing of order 3 at $y=0$ since $f(s,0,0) = \partial_y\omega_0(s,0) = \partial_y^2\omega_0(s,0) = 0$ when $t \in I$ by Propositions 3.4 and 4.2. Thus

$$R(s,y) = \mathcal{O}(|y|^3) = \mathcal{O}(\lambda^{-3\varrho}) = \mathcal{O}(\lambda^{-\varepsilon}) \quad \text{when } |y| \le c\lambda^{-\varrho},$$

since $\varrho = \varepsilon/3$. Now one loses at most a factor $y = \mathcal{O}(\lambda^{-\varrho}) = \mathcal{O}(\lambda^{-\varepsilon/3})$ when taking a derivative of $R(s,y)$, giving a factor $\mathcal{O}(\lambda^{\varrho})$, so $R(s,y) \in S(\lambda^{-\varepsilon}, g_\varrho)$.

It remains to consider the first three terms in (5.6) and as before it suffices to consider derivatives of order less than 3 at $y=0$. Since $\partial_y^3\omega_0(s,0) \in C^\infty$ uniformly we only have to estimate $\partial_\eta \operatorname{Im} f(s,0,0)$ and $\partial_{s,y}^k \operatorname{Im} f(s,0,0)$ when $k \le 2$. We obtain from (3.20) that

$$\partial_\eta \operatorname{Im} f(s,0,0) = \lambda^{3\varepsilon}\partial_\xi \operatorname{Im} r(t,0,\xi_0) = \mathcal{O}(\lambda^{-5\varepsilon/3}) = \mathcal{O}(\lambda^{-\varepsilon+2\varrho})$$

Similarly, (3.20) gives

$$\partial_{s,y} \operatorname{Im} f(s,0,0) = \lambda^{4\varepsilon}\partial_{t,x} \operatorname{Im} r(t,0,\xi_0) = \mathcal{O}(\lambda^{-2\varepsilon/3}) = \mathcal{O}(\lambda^{-\varepsilon+\varrho}),$$

and (3.21) gives

$$\partial_{s,y}^2 \operatorname{Im} f(s,0,0) = \lambda^{\varepsilon}\partial_{t,x}^2 \operatorname{Im} r(t,0,\xi_0) = \mathcal{O}(\lambda^{-\varepsilon/3}) = \mathcal{O}(\lambda^{-\varepsilon+2\varrho}). \qquad \square$$

By a change of t variable we may assume that (3.2) and (3.5) hold with the integration starting at $t=0$. We obtain new variables z in $\mathbf{R}^{n-1}$ by solving

$$\partial_t z_j = \langle a_j(t), z\rangle, \quad z_j(0) = x_j \quad \forall\, j.$$

Then $D_t + \sum_j \langle a_j(t), x\rangle D_{x_j}$ is transformed into D_t but $D_{x_j} = D_{z_j}$ is unchanged, and we will for simplicity keep the notation (t,x). The linear change of variables is uniformly bounded since $a_j \in C^\infty$, so it preserves the neighborhoods $|x| \lesssim \lambda^{-\nu}$ and the symbol classes $S(\lambda^\mu, g_\nu)$, $\forall\, \mu, \nu$. We shall then solve the approximate transport equation

$$D_t\varphi + (q_0(t) + ir_0(t,x))\varphi = 0 \tag{5.7}$$

where $\varphi(0,x) \in S(1,g_\delta)$ is supported where $|x| \lesssim \lambda^{-\delta}$, $q_0(t)$ is given by (5.3) and r_0 by (5.2). If we assume $3\varepsilon \le \delta \le 7\varepsilon/2$ then by Lemma 5.1 the approximation errors $R\varphi$ will be in $S(\lambda^{3\varepsilon-\delta}, g_\delta)$. In fact, since ∂_x maps $S(1,g_\delta)$ into $S(\lambda^\delta, g_\delta)$ we find $R(t,x,D_x)\varphi_0 \in S(\lambda^{3\varepsilon-\delta}, g_\delta)$ when $|x| \lesssim \lambda^{-\delta}$. We find from Proposition 3.1 that $q_0 \in S(\lambda^\varepsilon, g_\varepsilon)$, and if $\varepsilon = 1/8$ and $\delta = (1+2\varepsilon)/3$ then we find from Lemma 5.2 that $r_0 \in S(1,g_\delta)$ when $|x| \lesssim \lambda^{-\delta}$ and $t \in I$.

If we choose the initial data $\varphi(0,x) = \phi_0(x) = \phi(\lambda^\delta x)$, where $\phi \in C_0^\infty$ satisfies $\phi(0) = 1$, we obtain the solution

$$\varphi(t,x) = \phi_0(x)\exp(-iB(t,x)) \tag{5.8}$$

where $\partial_t B(t,x) = q_0(t) + ir_0(t,x)$ and $B(0,x) = 0$. We find that $\exp(-iB(t,x)) \in S(1, g_\delta)$ uniformly since condition (3.2) holds with $a_j \equiv 1$,

$$\partial_t B(t,x) = q_0(t) + ir_0(t,x) \in S(\lambda^\varepsilon, g_\varepsilon) + S(1, g_\delta) \subset S(\lambda^\delta, g_\delta)$$

and

$$\partial_x B(t,x) = i\int_0^t \partial_x r_0(s,x)\,ds \in S(\lambda^\delta, g_\delta)$$

by Proposition 3.1 and Lemma 5.2. Thus $\varphi \in S(1, g_\delta)$ uniformly and we find by (5.8) that $|\varphi(t,x)| \le C|\phi(\lambda^\delta x)|$ so $|x| \lesssim \lambda^{-\delta}$ in $\operatorname{supp}\varphi$, which also holds in the original x coordinates.

After solving the eikonal equation and the approximate transport equation, we find from Proposition 3.5 that the terms in the expansion (3.33) are $\mathcal{O}(\lambda^{3\varepsilon-\delta})$ if $\varepsilon < 1/7$ and $\delta = (1+2\varepsilon)/3$, and all the terms contain the factor $\exp(-iB(t,x))$. We take $\varepsilon = 1/8$ and $\delta = 5/12$ which gives $3\varepsilon - \delta = -1/24 > -\varepsilon/2$ so $3\varepsilon < \delta < 7\varepsilon/2$. Then the expansion in Proposition 3.5 is in multiples of $\lambda^{-1/24}$, and since the error terms of (3.35) are $\mathcal{O}(\lambda^{-1/24})$ we will take $\varrho = 1/24$ and $\varphi_0 = \varphi$ in the definition of u_λ given by (3.31).

The approximate transport equation for φ_k in (3.31), $k > 0$, is

$$D_t\varphi_k + (q_0(t) + ir_0(t,x))\varphi_k = \lambda^{k/24} R_k \exp(iB(t,x)), \quad k \ge 1, \tag{5.9}$$

with R_k is uniformly bounded in the symbol class $S(\lambda^{-k/24}, g_{5/12})$ and is supported where $|x| \lesssim \lambda^{-5/12}$. In fact, R_k contains the error terms from the transport equation (5.1) and also the terms that are $\mathcal{O}(\lambda^{-k/24})$ in (3.33) depending on φ_j for $j < k$. Taking $\varphi_k = \exp(-iB(t,x))\phi_k$ we obtain the equation

$$D_t\phi_k = \lambda^{k/24} R_k \in S(1, g_{5/12}) \tag{5.10}$$

with initial values $\phi_k(0,x) = 0$, which can be solved with $\phi_k \in S(1, g_{5/12})$ uniformly having support where $|x| \lesssim \lambda^{-5/12}$. Since $\exp(-iB(t,x)) \in S(1, g_{5/12})$ uniformly we find that $\varphi_k \in S(1, g_{5/12})$ uniformly having support where $|x| \lesssim \lambda^{-5/12}$. Proceeding by induction we obtain a solution to (3.33) modulo $\mathcal{O}(\lambda^{-N/24})$ for any N.

Proposition 5.3. *Assuming Propositions* 3.3 *and* 3.4 *and choosing* $\varepsilon = 1/8$, $\delta = 5/12$ *and* $\varrho = 1/24$ *we can solve the transport equations* (5.7) *and* (5.9) *with* $\varphi_k \in S(1, g_{5/12})$ *having support where* $|x| \lesssim \lambda^{-5/12}$*, such that* $\varphi_0(0,0) = 1$ *and* $\varphi_k(0,x) \equiv 0$*,* $k \ge 1$.

Now, we get localization in x from the initial values and the transport equation. To get localization in t we use that $\operatorname{Im} B(t) \le C$ so that $\operatorname{Re}(-iB) \le C$. Near $\partial\Gamma$ we may assume that $\operatorname{Re}(-iB(t)) \ll -\log\lambda$ in an interval of length $\mathcal{O}(\lambda^{-\varepsilon}) = \mathcal{O}(\lambda^{-1/8})$ by (3.5). Thus by applying a cut-off function $\chi(t) \in S(1, \lambda^{1/4}dt^2) \subset$

$S(1, g_{5/12})$ such that $\chi(0) = 1$ and $\chi'(t)$ is supported where (3.5) holds, i.e., where $\varphi_k = \mathcal{O}(\lambda^{-N})$, $\forall\, k$, we obtain a solution modulo $\mathcal{O}(\lambda^{-N})$ for any N. In fact, if u_λ is defined by (3.31) and Q by Proposition 3.3 then $Q\chi u_\lambda = \chi Q u_\lambda + [Q, \chi]u_\lambda$ where $[Q, \chi] = D_t\chi$ is supported where $u_\lambda = \mathcal{O}(\lambda^{-N})$ which gives terms that are $\mathcal{O}(\lambda^{-N})$, $\forall\, N$. Thus, by solving the eikonal equation (4.1) for ω and the transport equations (5.9) for φ_k for $k \le 24N$, we obtain that $Q\chi u_\lambda = \mathcal{O}(\lambda^{-N})$ for any N and we get the following remark.

Remark 5.4. In Proposition 5.3 we may assume that

$$\varphi_k(t, x) = \phi_k(\lambda^{5/12}t, \lambda^{5/12}x) \in S(1, g_{5/12}), \quad k \ge 0,$$

with $\phi_k \in C_0^\infty$ having support where $|x| \lesssim 1$ and $|t| \lesssim \lambda^{5/12}$, $k \ge 0$.

6. The proof of Theorem 2.11

For the proof we will need the following modification of [5, Lemma 26.4.14] which is Lemma 7.1 in [2]. Recall that $\mathcal{D}'_\Gamma = \{\, u \in \mathcal{D}' : \mathrm{WF}(u) \subset \Gamma \,\}$ for $\Gamma \subset T^*\mathbf{R}^n$, and that $\|u\|_{(k)}$ is the L^2 Sobolev norm of order k of $u \in C_0^\infty$.

Lemma 6.1. *Let*

$$u_\lambda(x) = \lambda^{(n-1)\delta/2} \exp(i\lambda^\varrho \omega(\lambda^\varepsilon x)) \sum_{j=0}^{M} \varphi_j(\lambda^\delta x)\lambda^{-j\kappa} \tag{6.1}$$

with $\omega \in C^\infty(\mathbf{R}^n)$ satisfying $\operatorname{Im}\omega \ge 0$ and $|d\omega| \ge c > 0$, $\varphi_j \in C_0^\infty(\mathbf{R}^n)$, $\lambda \ge 1$, ε, δ, κ, and ϱ are positive such that $\varepsilon < \delta < \varepsilon + \varrho$. Here ω and φ_j may depend on λ but uniformly, and φ_j has fixed compact support in all but one of the variables, for which the support is bounded by $C\lambda^\delta$. Then for any integer N we have

$$\|u_\lambda\|_{(-N)} \le C\lambda^{-N(\varepsilon+\varrho)}. \tag{6.2}$$

If $\varphi_0(x_0) \ne 0$ and $\operatorname{Im}\omega(x_0) = 0$ for some x_0 then there exists $c > 0$ and $\lambda_0 \ge 1$ so that

$$\|u_\lambda\|_{(-N)} \ge c\lambda^{-(N+\frac{n}{2})(\varepsilon+\varrho)+(n-1)\delta/2}, \quad \lambda \ge \lambda_0. \tag{6.3}$$

Let $\Sigma = \bigcap_{\lambda \ge 1} \bigcup_j \operatorname{supp}\varphi_j(\lambda\,\cdot)$ and let Γ be the cone generated by

$$\{\, (x, \partial\omega(x)),\ x \in \Sigma,\ \operatorname{Im}\omega(x) = 0 \,\}, \tag{6.4}$$

then for any real m we find $\lambda^m u_\lambda \to 0$ in $\mathcal{D}'_\Gamma$ so $\lambda^m A u_\lambda \to 0$ in C^∞ if A is a pseudodifferential operator such that $\mathrm{WF}(A) \cap \Gamma = \emptyset$. The estimates are uniform if $\omega \in C^\infty$ uniformly with fixed lower bound on $|d\operatorname{Re}\omega|$, and $\varphi_j \in C^\infty$ uniformly.

We shall use Lemma 6.1 for u_λ in (3.31), then ω will be real valued and Γ in (6.4) will be the bicharacteristic Γ_j converging to a limit bicharacteristic.

Proof of Lemma 6.1. We shall adapt the proof of [5, Lemma 26.4.14] to this case. By making the change of variables $y = \lambda^\varepsilon x$ we find that

$$\hat{u}_\lambda(\xi) = \lambda^{(n-1)\delta/2-n\varepsilon} \sum_{j=0}^{M} \lambda^{-j\kappa} \int e^{i(\lambda^\varrho \omega(y) - \langle y, \xi/\lambda^\varepsilon \rangle)} \varphi_j(\lambda^{\delta-\varepsilon} y)\, dy. \tag{6.5}$$

Let U be a neighborhood of the projection on the second component of the set in (6.4). When $\xi/\lambda^{\varepsilon+\varrho} \notin U$, then for $\lambda \gg 1$ we have that

$$\bigcup_j \operatorname{supp} \varphi_j(\lambda^{\delta-\varepsilon} \cdot) \ni y \mapsto (\lambda^\varrho \omega(y) - \langle y, \xi/\lambda^\varepsilon \rangle)/(\lambda^\varrho + |\xi|/\lambda^\varepsilon)$$
$$= (\omega(y) - \langle y, \xi/\lambda^{\varepsilon+\varrho} \rangle)/(1 + |\xi|/\lambda^{\varepsilon+\varrho})$$

is in a compact set of functions with non-negative imaginary part with a fixed lower bound on the gradient of the real part. Thus, by integrating by part in (6.5) we find for any positive integer m that

$$|\hat{u}_\lambda(\xi)| \le C_m \lambda^{-(n-1)\delta/2+m(\delta-\varepsilon)} (\lambda^\varrho + |\xi|/\lambda^\varepsilon)^{-m}, \quad \xi/\lambda^{\varepsilon+\varrho} \notin U,\ \lambda \gg 1. \tag{6.6}$$

This gives any negative power of λ for m large enough since $\delta < \varepsilon + \varrho$. If V is bounded and $0 \notin \overline{V}$ then since u_λ is uniformly bounded in L^2 we find

$$\int_{\tau V} |\hat{u}_\lambda(\xi)|^2 (1 + |\xi|^2)^{-N}\, d\xi \le C_V \tau^{-2N}, \quad \tau \ge 1.$$

Using this estimate with $\tau = \lambda^{\varepsilon+\varrho}$ together with the estimate (6.6) we obtain (6.2). If $\chi \in C_0^\infty$ then we may apply (6.6) to χu_λ, thus we find for any positive integer j that

$$|\widehat{\chi u}_\lambda(\xi)| \le C_j \lambda^{-(n-1)\delta/2+j(\delta-\varepsilon)} (\lambda^\varrho + |\xi|/\lambda^\varepsilon)^{-j}, \quad \xi \in W,\ \lambda \gg 1,$$

if W is any closed cone with $\Gamma \cap (\operatorname{supp} \chi \times W) = \emptyset$. Thus we find that $\lambda^m u_\lambda \to 0$ in $\mathcal{D}'_\Gamma$ for every m. To prove (6.3) we assume $x_0 = 0$ and take $\psi \in C_0^\infty$. If $\operatorname{Im} \omega(0) = 0$ and $\varphi(0) \neq 0$ we find

$$\lambda^{n(\varepsilon+\varrho)-(n-1)\delta/2} e^{-i\lambda^\varrho \operatorname{Re} \omega(0)} \langle u_\lambda, \psi(\lambda^{\varepsilon+\varrho} \cdot) \rangle$$
$$= \int e^{i\lambda^\varrho(\omega(x/\lambda^\varrho) - \omega(0))} \psi(x) \sum_j \varphi_j(x/\lambda^{\varepsilon+\varrho-\delta}) \lambda^{-j\kappa}\, dx$$
$$\to \int e^{i\langle \operatorname{Re} \partial_x \omega(0), x \rangle} \psi(x) \varphi_0(0)\, dx, \quad \text{as } \lambda \to +\infty,$$

which is not equal to zero for some suitable $\psi \in C_0^\infty$. In fact, we have

$$\varphi_j(x/\lambda^{\varepsilon+\varrho-\delta}) = \varphi_j(0) + \mathcal{O}(\lambda^{\delta-\varepsilon-\varrho}) \to \varphi_j(0)$$

when $\lambda \to \infty$, because $\delta < \varepsilon + \varrho$. Since

$$\|\psi(\lambda^{\varepsilon+\varrho} \cdot)\|_{(N)} \le C \lambda^{(N-n/2)(\varepsilon+\varrho)},$$

we obtain that $0 < c \le \lambda^{(N+\frac{n}{2})(\varepsilon+\varrho)-(n-1)\delta/2} \|u\|_{(-N)}$ which gives (6.3) and the lemma. ∎

Proof of Theorem 2.11. Assume that Γ is a limit bicharacteristic of P. We are going to show that (2.23) does not hold for any ν, N and any pseudodifferential operator A such that $\Gamma \cap \mathrm{WF}(A) = \emptyset$. This means that there exists $0 \neq u_j \in C_0^\infty$ such that

$$\|u_j\|_{(-N)}/(\|P^* u_j\|_{(\nu)} + \|u_j\|_{(-N-n)} + \|Au_j\|_{(0)}) \to \infty \quad \text{when } j \to \infty, \tag{6.7}$$

which will contradict the local solvability of P at Γ by Remark 2.12.

Let $\Gamma_j \subset \Sigma \cap S^*X$ be a sequence of semibicharacteristics of p that converges to the limit bicharacteristic $\Gamma \subset \Sigma_2$ and let λ_j be given by (2.10) and (3.4) with $\varepsilon > 0$ which will be chosen later. Now the conditions and conclusions are invariant under symplectic changes of homogeneous coordinates and multiplication by elliptic pseudodifferential operators. By Proposition 3.3 we may assume that the coordinates are chosen so that $\Gamma_j = I \times (0, 0, \xi_j)$ with $|\xi_j| = 1$, and for any $0 < \varepsilon < 1/3$ and $c > 0$ we can write $B_j P^* = Q_j + R_j \in \Psi^{1-\varepsilon}_{1-\varepsilon,\varepsilon}$ where $B_j \in \Psi^{\varepsilon}_{1-\varepsilon,\varepsilon}$ uniformly, $\Gamma_j \cap \mathrm{WF}_\varepsilon(R) = \emptyset$ uniformly and Q_j has symbol

$$\tau - r(t, x, \xi) + q_0(t, x, \xi) + r_0(t, x, \xi) \tag{6.8}$$

when the homogeneous distance to Γ_j is less than $c|\xi|^{-\varepsilon} \lesssim \lambda_j^{-\varepsilon}$. We have that $r_0 \in S^{3\varepsilon-1}_{1-\varepsilon,\varepsilon}$, $q_0 \in S^{\varepsilon}_{1-\varepsilon,\varepsilon}$ is given by (3.26), and $r \in S^{1-\varepsilon}_{1-\varepsilon,\varepsilon}$ with real part vanishing of second order at Γ_j, and the bounds are uniform in the symbol classes.

Now, we may replace the norms $\|u\|_{(s)}$ in (6.7) by the norms

$$\|u\|_s^2 = \|\langle D_x\rangle^s u\|^2 = \int \langle\xi\rangle^{2s} |\hat{u}(\tau, \xi)|^2 \, d\tau d\xi$$

and the corresponding spaces H_s. In fact, the quotient $\langle\xi\rangle/\langle(\tau, \xi)\rangle \cong 1$ when $|\tau| \lesssim |\xi|$, thus in a conical neighborhood of Γ. So replacing the norms in the estimate (6.7) only changes the constant and the operator A in the estimate (2.23). By using Proposition 3.4 we may assume that the grazing Lagrangean space $L_j(w) \equiv \{\, (s, y; 0, 0) : (s, y) \in \mathbf{R}^n \,\}$, $\forall\, w \in \Gamma_j$, after conjugation with a uniformly bounded C^1-section $F(t)$ of homogeneous Fourier integral operators, then $\partial_x^2 \operatorname{Re} r = 0$ at Γ_j. Observe that for each t we find that $F(t)$ is uniformly continuous in local H_s spaces, which we may use in (6.7) after changing A. Also the conjugation of $F(t)$ with the operator with symbol (6.8) has a uniformly bounded expansion. In fact, this follows since $t \mapsto F(t) \in C^1$ are homogeneous Fourier integral operators in the x variables and these preserve the symbol classes. By changing A again, we may then replace the local $\|u\|_s$ norms by the norms $\|u\|_{(s)}$ in (6.7) so that we can use Lemma 6.1.

Now, by choosing $\delta = 5/12$, $\varepsilon = 1/8$ and $\varrho = 1/24$ and using Propositions 3.5, 4.2, 5.3 and Remark 5.4, we can for each Γ_j construct approximate solution u_{λ_j} on the form (3.31) so that $Qu_{\lambda_j} = \mathcal{O}(\lambda_j^{-k})$, for any k. The real valued phase function is equal to $\langle x, \xi_j\rangle + \omega_j(t, x)$ where $|\xi_j| = 1$ and $\omega_j(t, x) \in S({\lambda_j}^{-7/8}, g_{3/8})$ and the values of

$$(t, x; \lambda_j \partial_t \omega_j(t, x), \lambda_j(\xi_j + \partial_x \omega_j(t, x)))$$

have homogeneous distance $\lesssim \lambda_j^{-5/12}$ to the rays through Γ_j when $|x| \lesssim {\lambda_j}^{-5/12}$, thus on $\operatorname{supp} u_{\lambda_j}$. Observe that if $\lambda_j \gg 1$ then we have that $|\xi_0 + \partial_x \omega_j(t,x)| \cong 1$ in $\operatorname{supp} u_{\lambda_j}$. In fact, we have

$$\omega_j(t,x) = {\lambda_j}^{-7/8} \widetilde{\omega}_j({\lambda_j}^{3/8}t, {\lambda_j}^{3/8}x)$$

where $\widetilde{\omega}_j \in C^\infty$ uniformly so $\partial_x \omega_j = \mathcal{O}(\lambda_j^{-1/2})$. Now

$$\lambda_j(\langle x, \xi_j \rangle + \omega_j(t,x)) = {\lambda_j}^{5/8} \langle {\lambda_j}^{3/8}x, \xi_j \rangle + {\lambda_j}^{1/8} \widetilde{\omega}_j({\lambda_j}^{3/8}t, {\lambda_j}^{3/8}x)$$

when $|x| \lesssim \lambda_j^{-5/12}$, thus $\delta = 5/12$, $\varrho = 5/8$, $\varepsilon = 3/8$ and $\kappa = 1/24$ in (6.1) so $\varepsilon + \varrho = 1 > \delta > \varepsilon$.

The amplitude functions for u_{λ_j} are $\varphi_{k,j}(t,x) = \phi_{k,j}({\lambda_j}^{5/12}t, {\lambda_j}^{5/12}x)$ where $\phi_{k,j} \in C_0^\infty$ uniformly in j with fixed compact support in x, but in t the support is bounded by $C{\lambda_j}^{5/12}$. Thus u_{λ_j} will satisfy the conditions in Lemma 6.1 uniformly. Clearly differentiation of Qu_{λ_j} can at most give a factor λ_j since $\delta < \varepsilon + \varrho = 1$. Because of the bound on the support of u_{λ_j} we may obtain that

$$\|Qu_{\lambda_j}\|_{(\nu)} = \mathcal{O}(\lambda_j^{-N-n}) \tag{6.9}$$

for any given ν.

If $\mathrm{WF}(A) \cap \Gamma = \emptyset$, then we find $\mathrm{WF}(A) \cap \Gamma_j = \emptyset$ for large j, so Lemma 6.1 gives $\|Au_{\lambda_j}\|_{(0)} = \mathcal{O}(\lambda_j^{-N-n})$ when $j \to \infty$. On $\operatorname{supp} u_{\lambda_j}$ we have $x = \mathcal{O}(\lambda_j^{-5/12})$ so the values of $(t, x; \lambda_j \partial_t \omega_j(t,x), \lambda_j(\xi_j + \partial_x \omega_j(t,x)))$ have homogeneous distance $\lesssim \lambda_j^{-5/12}$ to the rays through Γ_j. Thus, if $R_j \in S^{9/8}_{7/8,1/8}$ such that $\mathrm{WF}_{1/8}(R_j) \cup \Gamma_j = \emptyset$ uniformly then we find from the expansion (3.32) that all the terms of $R_j u_{\lambda_j}$ vanish for large enough λ_j. In fact, since $\lambda_j^{-5/12} \ll \lambda_j^{-1/8}$ for $j \gg 1$, we find for any α and K that

$$\partial^\alpha R_j(t, x; \lambda_j((0, \xi_j) + \partial_{t,x} \omega_j(t,x))) = O(\lambda_j^{-K})$$

in $\bigcup_k \operatorname{supp} \varphi_{k,j}$. As before, we find that $\|R_j u_{\lambda_j}\|_{(\nu)} = \mathcal{O}(\lambda_j^{-N-n})$ by the bound on the support of u_{λ_j}, so we obtain from (6.9) that

$$\|P^* u_{\lambda_j}\|_{(\nu)} = \mathcal{O}(\lambda_j^{-N-n}) \tag{6.10}$$

for any given ν.

Since $\varepsilon + \varrho = 1$ and $\delta > 0$ we also find from Lemma 6.1 that

$$\lambda_j^{-N} = \lambda_j^{-N(\varepsilon+\varrho)} \gtrsim \|u_{\lambda_j}\|_{(-N)} \gtrsim \lambda_j^{-(N+\frac{n}{2})(\varepsilon+\varrho)+(n-1)\delta/2} \geq \lambda_j^{-N-n/2}$$

when $\lambda_j \geq 1$. We obtain that (6.7) holds for $u_j = u_{\lambda_j}$ when $j \to \infty$, so Remark 2.12 gives that P is not solvable at the limit bicharacteristic Γ. ☐

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Quantization of Gaussians

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Dedicated to the memory of Boris Pavlov.

Abstract. Our paper is devoted to the oscillator semigroup, which can be defined as the set of operators whose kernels are centered Gaussian. Equivalently, they can be defined as the Weyl quantization of centered Gaussians. We use the Weyl symbol as the main parametrization of this semigroup. We derive formulas for the tracial and operator norm of the Weyl quantization of Gaussians. We identify the subset of Gaussians, which we call *quantum degenerate*, where these norms have a singularity.

1. Introduction

Throughout our paper we will use the Weyl quantization, which is the most natural correspondence between quantum and classical states. For a function $k = k(x, p)$, with $x, p \in \mathbb{R}^d$, we will denote by $\mathrm{Op}(k)$ its Weyl quantization. Then function k is called the Weyl symbol (or the Wigner function) of the operator $\mathrm{Op}(k)$.

The Heisenberg uncertainty relation says that one cannot compress a state both in position and momentum without any limits. This is different than in classical mechanics, where in principle a state can have no dispersion both in position and momentum.

One can ask what happens to a quantum state when we compress its Weyl symbol. To be more precise, consider the Gaussian function $\mathrm{e}^{-\lambda(x^2+p^2)}$, where $\lambda > 0$ is an arbitrary parameter that controls the "compression". It is easy to compute the Weyl quantization of $\mathrm{e}^{-\lambda(x^2+p^2)}$ and express it in terms of the quantum harmonic oscillator

$$H = \hat{x}^2 + \hat{p}^2 = \sum_{j=1}^{d} (\hat{x}_j^2 + \hat{p}_j^2). \tag{1.1}$$

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There are 3 distinct regimes of the parameter λ:

$$\mathrm{Op}\Big(\mathrm{e}^{-\lambda(x^2+p^2)}\Big) = \begin{cases} (1-\lambda^2)^{-d/2}\exp\Big[-\frac{1}{2}\log\frac{(1+\lambda)}{(1-\lambda)}H\Big], & 0<\lambda<1, \\ 2^{-d}\mathbb{1}_{\{d\}}(H), & \lambda=1, \\ (\lambda^2-1)^{-d/2}(-1)^{(H-d)/2}\exp\Big[-\frac{1}{2}\log\frac{(1+\lambda)}{(\lambda-1)}H\Big], & 1<\lambda. \end{cases} \tag{1.2}$$

Thus, for $0<\lambda<1$, the quantization of the Gaussian is proportional to a thermal state of H. As λ increases to 1, it becomes "less mixed"–its "temperature" decreases. At $\lambda=1$ it becomes pure—its "temperature" becomes zero and it is the ground state of H. For $1<\lambda<\infty$, when we compress the Gaussian, it is no longer positive—due to the factor $(-1)^{(H-d)/2}$ it has eigenvalues with alternating signs. Besides, it becomes "more and more mixed", contrary to the naive classical picture.

Thus, at $\lambda=1$ we observe a kind of a "phase transition": For $0\leq\lambda<1$ the quantization of a Gaussian behaves more or less according to the classical intuition. For $1<\lambda$ the classical intuition stops to work—compressing the classical symbol makes its quantization more "diffuse".

It is easy to compute the trace of (1.2):

$$\mathrm{Tr}\,\mathrm{Op}\Big(\mathrm{e}^{-\lambda(x^2+p^2)}\Big) = \frac{1}{2^d\lambda^d}. \tag{1.3}$$

Evidently, (1.3) does not see the "phase transition" at $\lambda=1$. However, if we consider the trace norm, this phase transition appears—the trace norm of (1.2) is differentiable except at $\lambda=1$:

$$\mathrm{Tr}\,\Big|\mathrm{Op}\Big(\mathrm{e}^{-\lambda(x^2+p^2)}\Big)\Big| = \begin{cases} \dfrac{1}{2^d\lambda^d} & \lambda\leq 1, \\ \dfrac{1}{2^d}, & 1\leq\lambda. \end{cases} \tag{1.4}$$

Note that (1.4) can be viewed as a kind of quantitative "uncertainty principle".

Our paper is devoted to operators that can be written as the Weyl quantization of a (centered) Gaussian, more precisely, operators of the form $a\mathrm{Op}\big(\mathrm{e}^{-A}\big)$, where A is a quadratic form with a strictly positive real part and $a\in\mathbb{C}$. Such operators form a semigroup called the *oscillator semigroup*. We denote it by $\mathrm{Osc}_{++}\big(\mathbb{C}^{2d}\big)$. We also considered its subsemigroup, called the *normalized oscillator semigroup* and denoted $\mathrm{Osc}_{++}^{\mathrm{nor}}\big(\mathbb{C}^{2d}\big)$, which consists of operators

$$\pm\sqrt{\det(\mathbb{1}+A\theta)}\mathrm{Op}\big(\mathrm{e}^{-A}\big),$$

where θ is $-\mathrm{i}$ times the symplectic form ω.

The oscillator semigroup is closely related to the complex symplectic group $Sp\big(\mathbb{C}^{2d}\big)$. In particular, there exists a natural 2–1 epimorphism from $\mathrm{Osc}_{++}^{\mathrm{nor}}\big(\mathbb{C}^{2d}\big)$ onto $Sp_{++}\big(\mathbb{C}^{2d}\big)$, which is a certain natural subsemigroup of $Sp\big(\mathbb{C}^{2d}\big)$.

The oscillator semigroup is also closely related to the better known *metaplectic group*, denoted $Mp\big(\mathbb{R}^{2d}\big)$. The metaplectic group is generated by operators of the form $\pm\sqrt{\det(\mathbb{1}+B\omega)}\mathrm{Op}\big(\mathrm{e}^{\mathrm{i}B}\big)$, where B is a real symmetric matrix. There exists a natural 2–1 epimorphism from $Mp\big(\mathbb{R}^{2d}\big)$ to the real symplectic group $Sp\big(\mathbb{R}^{2d}\big)$. Not all elements of the metaplectic group can be written as Weyl quantizations of a Gaussian.

The situation with the oscillator semigroup is somewhat different than with the metaplectic group. All elements of the oscillator semigroup are quantizations of a Gaussian, however, not all of them correspond to a (complex) symplectic transformation. Those that do not correspond to quadratic forms A satisfying $\det(\mathbb{1}+A\theta)=0$. We call such quadratic forms "quantum degenerate". Classically, they are of course nondegenerate. Only their quantization is degenerate. In particular, for a quantum degenerate A, the operator $\mathrm{Op}\big(\mathrm{e}^{-A}\big)$ is not proportional to an element of $\mathrm{Osc}_{++}^{\mathrm{nor}}\big(\mathbb{C}^{2d}\big)$. The set of quantum degenerate matrices can be viewed as a place where some kind of a phase transition takes place in the oscillator semigroup. For instance, as we show in our paper, the trace norm of $\mathrm{Op}\big(\mathrm{e}^{-A}\big)$ depends smoothly on quantum nondegenerate A's, however, its smoothness typically breaks down at quantum degenerate A's.

It is also natural to mention another type of an oscillator semigroup, which we denote $\mathrm{Osc}_{+}\big(\mathbb{C}^{2d}\big)$. It is the semigroup generated by the operators of the form $a\mathrm{Op}\big(\mathrm{e}^{-A}\big)$, where $A\geq 0$. $\mathrm{Osc}_{+}\big(\mathbb{C}^{2d}\big)$ contains both $\mathrm{Osc}_{++}\big(\mathbb{C}^{2d}\big)$ and $Mp\big(\mathbb{R}^{2d}\big)$. It is in some sense the closure of $\mathrm{Osc}_{++}\big(\mathbb{C}^{2d}\big)$. We mention this semigroup only in passing, concentrating on $\mathrm{Osc}_{++}\big(\mathbb{C}^{2d}\big)$, which is easier, because, as we mentioned above, all elements of $\mathrm{Osc}_{++}\big(\mathbb{C}^{2d}\big)$ have Gaussian symbols. Note that the convenient notation $++$ for >0 and $+$ for ≥ 0, which we use, is borrowed from Howe [16].

Most of the time our discussion of the oscillator semigroup is representation independent (without invoking a concrete Hilbert space on which $\mathrm{Op}\big(\mathrm{e}^{-A}\big)$ acts). Perhaps the most obvious representation is the so-called Schrödinger representation, where the Hilbert space is $L^2\big(\mathbb{R}^d\big)$, $\hat{x}$ is identified with the operator of multiplication by x and $\hat{p}$ is $\frac{1}{\mathrm{i}}\partial_x$. Another possible representation is the Fock representation (or, which is essentially equivalent, the Bargmann–Fock representation, see, e.g., [11]). In both Schrödinger and Bargmann–Fock representations the oscillator semigroup consists of operators with centered Gaussian kernels.

Let us now discuss the literature on operators with Gaussian kernels, or equivalently, on quantizations of Gaussians. Probably, the best known reference on this subject is a paper [16] by Howe. In fact, we follow to some extent the terminology from [16]. His paper contains, for instance, a formula of composition of operators with Gaussian kernels, a criterion for positivity of such operators and the proof that there exists a 2–1 epimorphism from the normalized oscillator semigroup to a subsemigroup of $Sp\big(\mathbb{C}^{2d}\big)$. Howe works mostly in the Schrödinger representation. Instead of the Weyl symbol, he occasionally considers the so-called *Weyl transform*, which is essentially the Fourier transform of the Weyl symbol.

Another important work on the subject is a paper [15] by Hilgert, who realized that the oscillator semigroup is isomorphic to a semigroup described by Bargmann, Brunet and Kramer (see [2], [6], and [7]). Hilgert uses mostly the *Fock–Bargmann representation.*

The book of Folland [14] contains a chapter on the oscillator semigroup, which sums up the main points of [15] and [16].

The existence of the "phase transition" at quantum degenerate positive Gaussians has been known for quite a long time, where the earliest reference we could find is the paper [20] by Unterberger.

Our paper differs from [14, 15, 16] by using the Weyl quantization as the basic tool for the description of the oscillator semigroup. It is in some sense parallel to the presentation of the metaplectic group contained in [11, Sect. 10.3]. The Weyl quantization is in our opinion a natural tool in this context. First of all, it is symplectically invariant (unlike the Fock–Bargmann transform or the Schrödinger representation). Because of that, the analysis based on the Weyl quantization is particularly convenient and yields simple formulas. Secondly, the Weyl quantization allows us to make a direct contact with the quantum–classical correspondence principle. This semiclassical aspect is hidden when one uses the Weyl transform, which is also symplectically invariant.

An operation, that we introduce, which we find interesting is the product # in the set of symmetric matrices. More precisely, it is defined so that $\mathrm{Op}\big(\mathrm{e}^{-A}\big)\mathrm{Op}\big(\mathrm{e}^{-B}\big)$ is proportional to $\mathrm{Op}\big(-\mathrm{e}^{A\#B}\big)$. Whenever defined, # is associative, however it is not always well defined. # can be viewed as a semiclassical noncommutative distortion of the usual sum of square matrices. As we show, quantum nondegenerate matrices with a positive part form a semigroup, which is essentially isomorphic to the oscillator semigroup.

Among new results obtained in our paper, there is a formula for the absolute value of an operator $\mathrm{Op}\big(\mathrm{e}^{-A}\big)$, its trace norm and its operator norm.

There exists a close relationship between the set of complex matrices equipped with # and the complex symplectic group. This relationship is quite intricate–it is almost a bijection, after removing some exceptional elements in both sets. One of new results of our paper is a detailed description of this relationship, see in particular Theorem 18.

An interesting recent paper of Viola [21] gives a formula for the norm of an element of the oscillator semigroup. Our formula for $\big\|\mathrm{Op}\big(\mathrm{e}^{-A}\big)\big\|$ is in our opinion simpler than Viola's.

As an application of the formula for the trace norm of $\mathrm{Op}\big(\mathrm{e}^{-A}\big)$ we give a proof of the boundedness of the Weyl quantization with an explicit estimate of the of the operator norm. This result, which is a version of the so-called Calderon–Vaillancourt Theorem for the Weyl quantization, follows the ideas of Cordes [10] and Kato [18], however, the estimate of the norm seems to be new.

Elements of the oscillator semigroup can be viewed as exponentials of quantum quadratic Hamiltonians, that is $\mathrm{e}^{-\mathrm{Op}(H)}$, where H is a classical quadratic Hamiltonian with a positive real part. One example of such a Hamiltonian is

$\hat{H}_\psi := \mathrm{e}^{\mathrm{i}\psi}\hat{p}^2 + \mathrm{e}^{-\mathrm{i}\psi}\hat{x}^2$ for $|\psi| < \frac{\pi}{2}$, which is often called the *Davies harmonic oscillator*. It has been noted by a number of authors that this operator has interesting, often counterintuitive properties. In particular, [1] and [21] point out that $\mathrm{e}^{-z\hat{H}_\psi}$ can be defined as a bounded operator only for z that belong to a subset of the complex plane of a rather curious shape. We reproduce this result using methods developed in this article.

The oscillator semigroup provides a natural framework for a discussion of holomorphic semigroups $z \mapsto \mathrm{e}^{-z\mathrm{Op}(H)}$ associated with accretive quadratic Hamiltonians $\mathrm{Op}(H)$. We briefly discuss this issue at the end of our paper.

Finally, let us mention that one can explicitly compute the Weyl symbol of various functions of the harmonic oscillator, not only of its exponential. In particular, formulas in terms of special functions for the Weyl symbol of the resolvent of the harmonic oscillator can be found in [12]; see also [8], where the inverse of the harmonic oscillator is considered.

2. Notation

Let $L(\mathbb{C}^n)$ denote the set of $n \times n$ matrices. For $R \in L(\mathbb{C}^n)$ we will write $\overline{R}$, $R^{\#}$, resp. R^* for its complex conjugate, transpose, resp. Hermitian adjoint. Elements of $\mathbb{C}^n$ are represented by column matrices, so that for $v, w \in \mathbb{C}^n$ the (sesquilinear) scalar product of v and w can be denoted by v^*w.

By $\sigma(R)$ we will denote the spectrum of R.

We set

$$L^{\mathrm{reg}}(\mathbb{C}^n) := \{R \in L(\mathbb{C}^n) \mid R + \mathbb{1} \text{ is invertible}\}. \tag{2.1}$$

For $R \in L^{\mathrm{reg}}(\mathbb{C}^n)$, its *Cayley transform* is defined by

$$c(R) := (\mathbb{1} - R)(\mathbb{1} + R)^{-1}.$$

The Cayley transform is a bijection on $L^{\mathrm{reg}}(\mathbb{C}^n)$ and it is involutive, i.e.,

$$c(c(R)) = R. \tag{2.2}$$

For $A \in L(\mathbb{C}^n)$, we write $A > 0$, resp. $A \geq 0$ if

$$\begin{aligned} v^*Av > 0, \quad v \in \mathbb{C}^n, \quad v \neq 0, \\ \text{resp.} \quad v^*Av \geq 0, \quad v \in \mathbb{C}^n. \end{aligned} \tag{2.3}$$

$\mathrm{Sym}(\mathbb{R}^n)$, resp. $\mathrm{Sym}(\mathbb{C}^n)$ denotes the set of symmetric real, resp. complex $n \times n$ matrices. We also set

$$\mathrm{Sym}_+(\mathbb{R}^n) := \{A \in \mathrm{Sym}(\mathbb{R}^n) \mid A \geq 0\}, \tag{2.4}$$

$$\mathrm{Sym}_{++}(\mathbb{R}^n) := \{A \in \mathrm{Sym}(\mathbb{R}^n) \mid A > 0\}, \tag{2.5}$$

$$\mathrm{Sym}_+(\mathbb{C}^n) := \{A \in \mathrm{Sym}(\mathbb{C}^n) \mid \mathrm{Re}\, A \geq 0\}, \tag{2.6}$$

$$\mathrm{Sym}_{++}(\mathbb{C}^n) := \{A \in \mathrm{Sym}(\mathbb{C}^n) \mid \mathrm{Re}\, A > 0\}. \tag{2.7}$$

Note that $\mathrm{Sym}_{++}(\mathbb{C}^n)$ is sometimes called the (generalized) *Siegel upper half-plane*. It is sometimes denoted S_n or $\mathfrak{S}_n$ [16].

The following proposition can be found in [16]:

Proposition 1. *If* $A \in \mathrm{Sym}_{++}(\mathbb{C}^n)$*, then* A^{-1} *exists and belongs to* $\mathrm{Sym}_{++}(\mathbb{C}^n)$*.*

Proof. Let $A = A_\mathrm{r} + \mathrm{i}A_\mathrm{i}$ with $A_\mathrm{r} \in \mathrm{Sym}_{++}(\mathbb{R}^n)$, $A_\mathrm{i} \in \mathrm{Sym}(\mathbb{R}^n)$. Let $B := \sqrt{A_\mathrm{r}}$, $C := B^{-1}A_\mathrm{i}B^{-1}$. Then $A = B(\mathbb{1} + \mathrm{i}C)B$ and $A^{-1} = B^{-1}(\mathbb{1} + \mathrm{i}C)^{-1}B^{-1}$. Clearly, $(\mathbb{1} + \mathrm{i}C)^{-1} \in \mathrm{Sym}_{++}(\mathbb{C}^n)$. Hence $A^{-1} \in \mathrm{Sym}_{++}(\mathbb{C}^n)$. □

Every $n \times n$ symmetric matrix A defines a quadratic form on $\mathbb{R}^n$ by

$$\mathbb{R}^n \ni y \mapsto y^{\#}Ay \in \mathbb{C}. \tag{2.8}$$

We will often write A for the function (2.8). Thus, in particular,

$$\mathrm{e}^{-A}(y) = \mathrm{e}^{-y^{\#}Ay}.$$

We will often need to use the square root of a complex number a. If it is clear from the context that a is positive and real, then $\sqrt{a}$ will always denote the positive square root. If a is a priori arbitrary, then $\pm\sqrt{a}$ will denote both values of the square root. If a given formula involves only one of possible values of the square root, then we will write $\epsilon\sqrt{a}$ *where* $\epsilon = 1$ *or* $\epsilon = -1$.

3. The Weyl quantization

Recall that for any $k \in \mathscr{S}'\big(\mathbb{R}^d \times \mathbb{R}^d\big)$

$$\mathrm{Op}(k)(x, y) = (2\pi)^{-d} \int k\Big(\frac{x+y}{2}, p\Big)\mathrm{e}^{\mathrm{i}p(x-y)}\,\mathrm{d}p \tag{3.1}$$

is called the *Weyl–Wigner quantization of the symbol* k, see, e.g., [17, Sect. 18.5] or [11]. We can recover the symbol of a quantization from its distributional kernel by

$$k(x, p) = \int \mathrm{Op}(k)\Big(x + \frac{z}{2}, x - \frac{z}{2}\Big)\,\mathrm{e}^{-\mathrm{i}zp}\,\mathrm{d}z. \tag{3.2}$$

For sufficiently nice functions k, m we can define the *star product* $*$ (sometimes called the *Moyal star*) such that $\mathrm{Op}(k)\mathrm{Op}(m) = \mathrm{Op}(k * m)$ holds. On the level of symbols we have

$$(k * m)(x, p) := \mathrm{e}^{\frac{\mathrm{i}}{2}(\partial_{x_1}\partial_{p_2} - \partial_{p_1}\partial_{x_2})}k(x_1, p_1)m(x_2, p_2)\Big|_{\substack{x:=x_1=x_2\\ p:=p_1=p_2}}. \tag{3.3}$$

Write $y = \begin{bmatrix} x \\ p \end{bmatrix}$, $\omega := \begin{bmatrix} 0 & \mathbb{1}_d \\ -\mathbb{1}_d & 0 \end{bmatrix}$, and $\theta := \begin{bmatrix} 0 & -\mathrm{i}\mathbb{1}_d \\ \mathrm{i}\mathbb{1}_d & 0 \end{bmatrix} = -\mathrm{i}\omega$. One can rewrite (3.3) in a more compact form:

$$(k * m)(y) = \mathrm{e}^{-\frac{1}{2}\partial_{y_1}\theta\partial_{y_2}}k(y_1)m(y_2)\Big|_{y:=y_1=y_2}. \tag{3.4}$$

Here is an integral form of (3.4):

$$(k * m)(y) = \pi^{-2d}\int \mathrm{d}y_1 \int \mathrm{d}y_2\, \mathrm{e}^{2(y-y_1)\theta(y-y_2)}k(y_1)m(y_2), \tag{3.5}$$

(see, e.g., [11, Theorem 8.70(4)]). For the product of three symbols, we have

$$\begin{aligned}
&(k * m * n)(y) \\
&= \mathrm{e}^{-\frac{1}{2}\partial_{y_1}\theta\partial_{y_2}-\frac{1}{2}\partial_{y_1}\theta\partial_{y_3}-\frac{1}{2}\partial_{y_2}\theta\partial_{y_3}} k(y_1)m(y_2)n(y_3)\Big|_{y:=y_1=y_2=y_3} \\
&= \pi^{-3d}\int \mathrm{d}y_1 \int \mathrm{d}y_2 \int \mathrm{d}y_3\, \mathrm{e}^{(y-y_1)\theta(y-y_2)+(y-y_2)\theta(y-y_3)+(y-y_1)\theta(y-y_3)} \qquad (3.6)\\
&\quad \times \mathrm{e}^{-\frac{1}{2}(y-y_1)\theta(y-y_1)-\frac{1}{2}(y-y_2)\theta(y-y_2)-\frac{1}{2}(y-y_3)\theta(y-y_3)} k(y_1)m(y_2)n(y_3)\Big|_{y=y_1=y_2=y_3}.
\end{aligned}$$

4. Product

Let $A, B \in \mathrm{Sym}(\mathbb{C}^{2d})$. Suppose that

$$\text{the matrix } \begin{bmatrix} \theta A\theta & -\theta \\ \theta & \theta B\theta \end{bmatrix} \text{ is invertible.} \tag{4.1}$$

We then define $A\#B \in \mathrm{Sym}(\mathbb{C}^{2d})$ by

$$A\#B := \begin{bmatrix} -1\!\!1 \\ 1\!\!1 \end{bmatrix}^{\#} \begin{bmatrix} \theta A\theta & -\theta \\ \theta & \theta B\theta \end{bmatrix}^{-1} \begin{bmatrix} -1\!\!1 \\ 1\!\!1 \end{bmatrix}. \tag{4.2}$$

For the time being, the definition of the product # may seem strange. As we will soon see in Sect. 6, it is motivated by the product of operators with Gaussian symbols.

The following proposition gives a condition which guarantees that $A\#B$ is well defined.

Proposition 2. *Condition* (4.1) *holds iff the inverse of* $(1\!\!1 + A\theta B\theta)$ *exists. We then have*

$$\begin{aligned}
\begin{bmatrix} \theta A\theta & -\theta \\ \theta & \theta B\theta \end{bmatrix}^{-1} &= \begin{bmatrix} (\theta A\theta + B^{-1})^{-1} & (\theta + \theta B\theta A\theta)^{-1} \\ -(\theta + \theta A\theta B\theta)^{-1} & (\theta B\theta + A^{-1})^{-1} \end{bmatrix} \\
&= \begin{bmatrix} B\theta(1\!\!1 + A\theta B\theta)^{-1}\theta & (1\!\!1 + B\theta A\theta)^{-1}\theta \\ -(1\!\!1 + A\theta B\theta)^{-1}\theta & A\theta(1\!\!1 + B\theta A\theta)^{-1}\theta \end{bmatrix}, \qquad (4.3)\\
A\#B &= (\theta A\theta + B^{-1})^{-1} + (\theta B\theta + A^{-1})^{-1} \\
&\quad + (\theta + \theta A\theta B\theta)^{-1} - (\theta + \theta B\theta A\theta)^{-1}. \qquad (4.4)
\end{aligned}$$

Proof. It is well known how to compute an inverse of a 2×2 block matrix. This yields (4.3), which implies (4.4).

Clearly,

$$\theta(1\!\!1 + A\theta B\theta)^{\#}\theta = (1\!\!1 + B\theta A\theta). \tag{4.5}$$

Therefore, the inverse of $(1\!\!1 + A\theta B\theta)$ exists iff the inverse of $(1\!\!1 + B\theta A\theta)$ exists. If this is the case, then all terms in (4.3) and (4.4) are well defined. □

Proposition 3. *The product # is associative, i.e., if* $A, B, C \in \mathrm{Sym}\big(\mathbb{C}^{2d}\big)$ *and* $A\#B$, $B\#C$, $(A\#B)\#C$ *and* $A\#(B\#C)$ *are well defined, then*

$$(A\#B)\#C = A\#(B\#C). \tag{4.6}$$

Besides,

$$A\#0 = 0\#A = A, \qquad A\#(-A) = 0,$$
$$\overline{A\#B} = \overline{B}\#\overline{A}, \qquad (-A)\#(-B) = -B\#A.$$

Proof. We check that

$$\begin{aligned}(A\#B)\#C &= A\#(B\#C)\\ &= \begin{bmatrix}-\mathbb{1}\\0\\\mathbb{1}\end{bmatrix}^{\#}\begin{bmatrix}\theta A\theta+\frac12\theta & -\frac12\theta & -\frac12\theta\\ \frac12\theta & \theta B\theta+\frac12\theta & -\frac12\theta\\ \frac12\theta & \frac12\theta & \theta C\theta+\frac12\theta\end{bmatrix}^{-1}\begin{bmatrix}-\mathbb{1}\\0\\\mathbb{1}\end{bmatrix}.\end{aligned} \tag{4.7}$$

(Compare with (3.6)). This yields (4.6). The remaining statements are straightforward. □

Note that it is useful to think of # as a noncommutative deformation of the addition. In fact, we have

$$A\#B = A + B + O(A^2 + B^2). \tag{4.8}$$

5. Quantum non-degenerate matrices

Define

$$\mathrm{Sym}^{\mathrm{qnd}}\big(\mathbb{C}^{2d}\big) := \big\{A \in \mathrm{Sym}\big(\mathbb{C}^{2d}\big) \ : \ \det(\mathbb{1} + A\theta) \neq 0\big\}, \tag{5.1}$$
$$\mathrm{Sym}^{\mathrm{qnd}}_{++}\big(\mathbb{C}^{2d}\big) := \big\{A \in \mathrm{Sym}_{++}\big(\mathbb{C}^{2d}\big) \ : \ \det(\mathbb{1} + A\theta) \neq 0\big\}, \tag{5.2}$$
$$\mathrm{Sym}^{\mathrm{qnd}}\big(\mathbb{R}^{2d}\big) := \big\{A \in \mathrm{Sym}\big(\mathbb{R}^{2d}\big) \ : \ \det(\mathbb{1} + A\theta) \neq 0\big\}, \tag{5.3}$$
$$\mathrm{Sym}^{\mathrm{qnd}}_{++}\big(\mathbb{R}^{2d}\big) := \big\{A \in \mathrm{Sym}_{++}\big(\mathbb{R}^{2d}\big) \ : \ \det(\mathbb{1} + A\theta) \neq 0\big\}. \tag{5.4}$$

("qnd" stands for *quantum non-degenerate*).

There are several equivalent formulas for the product (4.2). It is actually not so obvious to pass from one of them to another. In the following proposition we give a few of them.

Proposition 4. *Let* $A, B \in \mathrm{Sym}^{\mathrm{qnd}}\big(\mathbb{C}^{2d}\big)$ *such that* $(\mathbb{1} + A\theta B\theta)^{-1}$ *exists. Then*

$$\begin{aligned}A\#B &= c\big(c(A\theta)c(B\theta)\big)\theta && (5.5)\\ &= (\mathbb{1}+A\theta)^{-1}(A\theta+B\theta)(\mathbb{1}+A\theta B\theta)^{-1}(\mathbb{1}+A\theta)\theta && (5.6)\\ &= (\mathbb{1}+B\theta)(\mathbb{1}+A\theta B\theta)^{-1}(A\theta+B\theta)(\mathbb{1}+B\theta)^{-1}\theta && (5.7)\\ &= (\mathbb{1}-A\theta)(\mathbb{1}+B\theta A\theta)^{-1}(A\theta+B\theta)(\mathbb{1}-A\theta)^{-1}\theta && (5.8)\\ &= (\mathbb{1}-B\theta)^{-1}(A\theta+B\theta)(\mathbb{1}+B\theta A\theta)^{-1}(\mathbb{1}-B\theta)\theta. && (5.9)\end{aligned}$$

We have

$$\mathbb{1} + A\theta B\theta = (\mathbb{1} + A\theta)(\mathbb{1} + A\#B\theta)^{-1}(\mathbb{1} + B\theta), \tag{5.10}$$

and $A\#B \in \mathrm{Sym}^{\mathrm{qnd}}\big(\mathbb{C}^{2d}\big)$.

Proof. To see (5.5), it is enough to show that

$$c(A\#B\theta) = c(A\theta)c(B\theta). \tag{5.11}$$

Equation (4.4) can be rewritten as

$$\begin{aligned} A\#B &= B\theta(\mathbb{1} + A\theta B\theta)^{-1}\theta + A\theta(\mathbb{1} + B\theta A\theta)^{-1}\theta \\ &\quad + (\mathbb{1} + A\theta B\theta)^{-1}\theta - (\mathbb{1} + B\theta A\theta)^{-1}\theta \\ &= (\mathbb{1} + B\theta)(\mathbb{1} + A\theta B\theta)^{-1}\theta - (\mathbb{1} - A\theta)(\mathbb{1} + B\theta A\theta)^{-1}\theta. \end{aligned}$$

Therefore,

$$\begin{aligned} \mathbb{1} - A\#B\theta &= (A\theta - \mathbb{1})B\theta(\mathbb{1} + A\theta B\theta)^{-1} + (\mathbb{1} - A\theta)(\mathbb{1} + B\theta A\theta)^{-1} \\ &= (\mathbb{1} - A\theta)(\mathbb{1} + B\theta A\theta)^{-1}(\mathbb{1} - B\theta); \end{aligned} \tag{5.12}$$

$$\begin{aligned} \mathbb{1} + A\#B\theta &= (\mathbb{1} + B\theta)A\theta(\mathbb{1} + B\theta A\theta)^{-1} + (\mathbb{1} + B\theta)(\mathbb{1} + A\theta B\theta)^{-1} \\ &= (\mathbb{1} + B\theta)(\mathbb{1} + A\theta B\theta)^{-1}(\mathbb{1} + A\theta). \end{aligned} \tag{5.13}$$

Hence,

$$\begin{aligned} &c(A\#B\theta) \\ &= (\mathbb{1} - A\theta)(\mathbb{1} + B\theta A\theta)^{-1}(\mathbb{1} - B\theta)(\mathbb{1} + A\theta)^{-1}(A\theta B\theta + \mathbb{1})(\mathbb{1} + B\theta)^{-1} \\ &= (\mathbb{1} - A\theta)(\mathbb{1} + B\theta A\theta)^{-1}(\mathbb{1} - B\theta)\big(B\theta + (\mathbb{1} + A\theta)^{-1}(\mathbb{1} - B\theta)\big)(\mathbb{1} + B\theta)^{-1} \\ &= (\mathbb{1} - A\theta)(\mathbb{1} + B\theta A\theta)^{-1}\big(B\theta + (\mathbb{1} - B\theta)(\mathbb{1} + A\theta)^{-1}\big)(\mathbb{1} - B\theta)(\mathbb{1} + B\theta)^{-1} \\ &= (\mathbb{1} - A\theta)(\mathbb{1} + B\theta A\theta)^{-1}(\mathbb{1} + B\theta A\theta)(\mathbb{1} + A\theta)^{-1}(\mathbb{1} - B\theta)(\mathbb{1} + B\theta)^{-1} \\ &= c(A\theta)c(B\theta). \end{aligned}$$

Thus (5.5) is proven.

Next note that

$$\begin{aligned} c(A\theta)c(B\theta) &= (\mathbb{1} + A\theta)^{-1}(\mathbb{1} - A\theta)(\mathbb{1} - B\theta)(\mathbb{1} + B\theta)^{-1} \\ &= (\mathbb{1} + A\theta)^{-1}(\mathbb{1} - A\theta - B\theta + A\theta B\theta)(\mathbb{1} + B\theta)^{-1}. \end{aligned} \tag{5.14}$$

Therefore,

$$\mathbb{1} - c(A\theta)c(B\theta) = 2(\mathbb{1} + A\theta)^{-1}(A\theta + B\theta)(\mathbb{1} + B\theta)^{-1} \tag{5.15}$$

$$\mathbb{1} + c(A\theta)c(B\theta) = 2(\mathbb{1} + A\theta)^{-1}(\mathbb{1} + A\theta B\theta)(\mathbb{1} + B\theta)^{-1}. \tag{5.16}$$

Next we insert (5.15) and (5.16) into

$$A\#B = c\big(c(A\theta)c(B\theta)\big)\theta \tag{5.17}$$

$$= \big(\mathbb{1} - c(A\theta)c(B\theta)\big)\big(\mathbb{1} + c(A\theta)c(B\theta)\big)^{-1}\theta \tag{5.18}$$

$$= \big(\mathbb{1} + c(A\theta)c(B\theta)\big)^{-1}\big(\mathbb{1} - c(A\theta)c(B\theta)\big)\theta, \tag{5.19}$$

obtaining (5.6), resp. (5.7).

We know that $A\#B$ is symmetric. Applying the transposition to (5.6), resp. (5.7), we obtain (5.8), resp. (5.9), where we use $\theta^{\#} = -\theta$, $A^{\#} = A$, $B^{\#} = B$.

Equation (5.10) is proven in (5.13). This implies that $\mathbb{1} + A\#B\theta$ is invertible. Hence $A\#B \in \mathrm{Sym}^{\mathrm{qnd}}(\mathbb{C}^{2d})$. □

The set $\mathrm{Sym}^{\mathrm{qnd}}(\mathbb{C}^{2d})$ equipped with (4.2) is not a semigroup. It is enough to see that for $A = B = \begin{bmatrix} \mathrm{i} & 0 \\ 0 & \mathrm{i} \end{bmatrix}$ we have $\mathbb{1} + A\theta B\theta = 0$, so $A\#B$ is not defined.

Proposition 5. $\mathrm{Sym}_{++}(\mathbb{C}^{2d})$ *is a semigroup.*

Proof. Let A and B belong to $\mathrm{Sym}_{++}(\mathbb{C}^{2d})$. The matrix $\begin{bmatrix} \theta A\theta & -\theta \\ \theta & \theta B\theta \end{bmatrix}$ belongs to $\mathrm{Sym}_{++}(\mathbb{C}^{2d})$. Hence, so does its inverse. Thus, (4.2) also belongs to $\mathrm{Sym}_{++}(\mathbb{C}^{2d})$. This shows that $A\#B$ is well defined and belongs to $\mathrm{Sym}_{++}(\mathbb{C}^{2d})$. □

Proposition 6. $\mathrm{Sym}_{++}^{\mathrm{qnd}}(\mathbb{C}^{2d})$ *is also a semigroup.*

Proof. Let A and B belong to $\mathrm{Sym}_{++}^{\mathrm{qnd}}(\mathbb{C}^{2d})$. We already know that $A\#B$ is well defined, and hence $\mathbb{1} + A\theta B\theta$ is invertible (see Proposition 2). Using (5.10) and the invertibility of $\mathbb{1} + A\theta$, $\mathbb{1} + B\theta$, we can conclude that $\mathbb{1} + A\#B\theta$ is invertible. Hence $A\#B \in \mathrm{Sym}_{++}^{\mathrm{qnd}}(\mathbb{C}^{2d})$. □

6. Oscillator semigroup

Following [16, 14], the *oscillator semigroup* $\mathrm{Osc}_{++}(\mathbb{C}^{2d})$ is defined as the set of operators on $L^2(\mathbb{R}^d)$ whose Weyl symbols are centered Gaussian, that is operators of the form $a\mathrm{Op}(\mathrm{e}^{-A})$, where $a \in \mathbb{C}$, $A \in \mathrm{Sym}_{++}(\mathbb{C}^{2d})$ and $A(x,p) = \begin{bmatrix} x \\ p \end{bmatrix}^{\#} A \begin{bmatrix} x \\ p \end{bmatrix}$. (In [16], this semigroup is denoted by Ω).

There are several equivalent characterizations of $\mathrm{Osc}_{++}(\mathbb{C}^{2d})$. Here is one of them:

Proposition 7. $\mathrm{Osc}_{++}(\mathbb{C}^{2d})$ *equals the set of operators on* $L^2(\mathbb{R}^d)$ *with centered Gaussian kernels. More precisely, the integral kernel of* $a\mathrm{Op}(\mathrm{e}^{-A})$ *for* $A = \begin{bmatrix} B & D \\ D^{\#} & F \end{bmatrix}$ *is* $c\mathrm{e}^{-C(x,y)}$, *where*

$$c = \frac{2^{-d}a}{\sqrt{\det(F)}}, \tag{6.1}$$

$$C(x,y) = -\frac{1}{4}\begin{bmatrix} x \\ y \end{bmatrix}^{\#} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} B - DF^{-1}D^{\#} & -\mathrm{i}DF^{-1} \\ -\mathrm{i}F^{-1}D^{\#} & F^{-1} \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix}$$
$$= -\frac{1}{4}\begin{bmatrix} x \\ y \end{bmatrix}^{\#} \begin{bmatrix} c_{11} & c_{12} \\ c_{21} & c_{22} \end{bmatrix} \begin{bmatrix} x \\ y \end{bmatrix},$$

and

$$\begin{aligned} c_{11} &= B - DF^{-1}D^{\#} - \mathrm{i}DF^{-1} - \mathrm{i}F^{-1}D^{\#} + F^{-1}, \\ c_{12} &= B - DF^{-1}D^{\#} + \mathrm{i}DF^{-1} - \mathrm{i}F^{-1}D^{\#} - F^{-1}, \\ c_{21} &= B - DF^{-1}D^{\#} - \mathrm{i}DF^{-1} + \mathrm{i}F^{-1}D^{\#} - F^{-1}, \\ c_{22} &= B - DF^{-1}D^{\#} + \mathrm{i}DF^{-1} + \mathrm{i}F^{-1}D^{\#} + F^{-1}. \end{aligned}$$

Proof. The formula follows by elementary Gaussian integration. The detailed computations can be found in [14]. □

Proposition 8. *Let A and B belong to $\mathrm{Sym}_{++}(\mathbb{C}^{2d})$. Then the following product formula holds:*

$$\mathrm{Op}(\mathrm{e}^{-A})\mathrm{Op}(\mathrm{e}^{-B}) = \frac{\epsilon}{\sqrt{\det(A\theta B\theta + \mathbb{1})}}\mathrm{Op}(\mathrm{e}^{-A\#B}), \tag{6.2}$$

where $\epsilon = 1$ or $\epsilon = -1$. Consequently, $\mathrm{Osc}_{++}(\mathbb{C}^{2d})$ is a semigroup and

$$\mathrm{Osc}_{++}(\mathbb{C}^{2d}) \ni c\mathrm{Op}(\mathrm{e}^{-A}) \mapsto A \in \mathrm{Sym}_{++}(\mathbb{C}^{2d}) \tag{6.3}$$

is an epimorphism.

Proof. Formula (3.5) assures us that

$$\begin{aligned} &(\mathrm{e}^{-y^{\#}Ay} * \mathrm{e}^{-y^{\#}By})(y) \\ &= \pi^{-2d}\int \mathrm{d}y_1 \int \mathrm{d}y_2 \exp\big(-2(y-y_2)\theta(y-y_1) - y_1^{\#}Ay_1 - y_2^{\#}By_2\big) \\ &= \pi^{-2d}\int \mathrm{d}y_1 \int \mathrm{d}y_2 \exp\left(-\begin{bmatrix} y_1 \\ y_2 \end{bmatrix}^{\#} \begin{bmatrix} A & -\theta \\ \theta & B \end{bmatrix} \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} - 2\begin{bmatrix} y_1 \\ y_2 \end{bmatrix}^{\#} \begin{bmatrix} -\theta y \\ \theta y \end{bmatrix}\right) \\ &= \det\begin{bmatrix} A & -\theta \\ \theta & B \end{bmatrix}^{-1/2} \exp\left(\begin{bmatrix} -\theta y \\ \theta y \end{bmatrix}^{\#} \begin{bmatrix} A & -\theta \\ \theta & B \end{bmatrix}^{-1} \begin{bmatrix} -\theta y \\ \theta y \end{bmatrix}\right). \end{aligned} \tag{6.4}$$

Then we check that

$$\det\begin{bmatrix} A & -\theta \\ \theta & B \end{bmatrix} = \det(\mathbb{1} + A\theta B\theta), \tag{6.5}$$

$$\begin{bmatrix} -\theta y \\ \theta y \end{bmatrix}^{\#} \begin{bmatrix} A & -\theta \\ \theta & B \end{bmatrix}^{-1} \begin{bmatrix} -\theta y \\ \theta y \end{bmatrix} = -\begin{bmatrix} -y \\ y \end{bmatrix}^{\#} \begin{bmatrix} \theta A\theta & -\theta \\ \theta & \theta B\theta \end{bmatrix}^{-1} \begin{bmatrix} -y \\ y \end{bmatrix}. \tag{6.6}$$

□

Again, following [16, 14], we introduce the *normalized oscillator semigroup*, denoted $\mathrm{Osc}^{\mathrm{nor}}_{++}(\mathbb{C}^{2d})$, as

$$\left\{\pm\sqrt{\det(\mathbb{1}+A\theta)}\mathrm{Op}\big(\mathrm{e}^{-A}\big) \mid A \in \mathrm{Sym}^{\mathrm{qnd}}_{++}(\mathbb{C}^{2d})\right\}.$$

(In [16], this semigroup is denoted by Ω^0).

Proposition 9. $\mathrm{Osc}^{\mathrm{nor}}_{++}(\mathbb{C}^{2d})$ *is a subsemigroup of* $\mathrm{Osc}_{++}(\mathbb{C}^{2d})$ *and*

$$\mathrm{Osc}^{\mathrm{nor}}_{++}(\mathbb{C}^{2d}) \ni \pm\sqrt{\det(\mathbb{1}+A\theta)}\mathrm{Op}\big(\mathrm{e}^{-A}\big) \mapsto A \in \mathrm{Sym}^{\mathrm{qnd}}_{++}(\mathbb{C}^{2d}) \tag{6.7}$$

is a 2–1 epimorphism of semigroups.

Proof. It is enough to check that

$$\begin{aligned}&\sqrt{\det(\mathbb{1}+A\theta)}\mathrm{Op}\big(\mathrm{e}^{-A}\big)\sqrt{\det(\mathbb{1}+B\theta)}\mathrm{Op}\big(\mathrm{e}^{-B}\big)\\ &=\epsilon\sqrt{\det(\mathbb{1}+A\#B\theta)}\mathrm{Op}\big(\mathrm{e}^{-A\#B}\big),\end{aligned} \tag{6.8}$$

where $\epsilon = 1$ or $\epsilon = -1$. Indeed, (5.10) implies

$$\det(\mathbb{1}+A\theta B\theta) = \det(\mathbb{1}+A\theta)\det(\mathbb{1}+A\#B\theta)^{-1}\det(\mathbb{1}+B\theta). \tag{6.9}$$

Now we need to use (6.2). □

7. Positive elements of the oscillator semigroup

We define

$$\mathrm{Sym}_{\mathrm{p}}(\mathbb{R}^{2d}) := \big\{A \in \mathrm{Sym}_{++}(\mathbb{R}^{2d}) \mid \sigma(A\theta) \subset [-1,1]\big\}, \tag{7.1}$$

$$\mathrm{Sym}^{\mathrm{qnd}}_{\mathrm{p}}(\mathbb{R}^{2d}) := \big\{A \in \mathrm{Sym}_{\mathrm{p}}(\mathbb{R}^{2d}) \mid \det(A\theta+\mathbb{1}) \neq 0\big\}. \tag{7.2}$$

Proposition 10. *Let* $a \in \mathbb{C}$ *and* $A \in \mathrm{Sym}_{++}(\mathbb{C}^{2d})$. *Then*

(1) $\big(a\mathrm{Op}(\mathrm{e}^{-A})\big)^* = \overline{a}\mathrm{Op}\big(\mathrm{e}^{-\overline{A}}\big)$.
(2) $a\mathrm{Op}\big(\mathrm{e}^{-A}\big)$ *is Hermitian iff* $a \in \mathbb{R}$ *and* $A \in \mathrm{Sym}_{++}(\mathbb{R}^{2d})$.
(3) $a\mathrm{Op}\big(\mathrm{e}^{-A}\big)$ *is positive iff* $a > 0$, $A \in \mathrm{Sym}_{\mathrm{p}}(\mathbb{R}^{2d})$.

Proof. Claims (1) and (2) follow from the obvious identity $\mathrm{Op}(a)^* = \mathrm{Op}(\overline{a})$.

Let us prove (3). A is a positive definite real matrix and ω is a symplectic matrix. It is well known, that they can be simultaneously diagonalized, that is, one can find a basis of $\mathbb{R}^{2d}$ such that if we write $\mathbb{R}^{2d} = \bigoplus_{i=1}^{d}\mathbb{R}^2$, then ω is the direct sum of $\begin{bmatrix}0 & 1\\ -1 & 0\end{bmatrix}$ and A is the direct sum of $\begin{bmatrix}\lambda_i & 0\\ 0 & \lambda_i\end{bmatrix}$ with $\lambda_i > 0$. After an appropriate metaplectic transformation, we can represent the Hilbert space $L^2(\mathbb{R}^d)$ as $\bigotimes_{i=1}^{d} L^2(\mathbb{R})$ and $\mathrm{Op}\big(\mathrm{e}^{-A}\big)$ can be represented as $\bigotimes_{i=1}^{d}\mathrm{Op}\Big(\mathrm{e}^{-\lambda_i(x_i^2+p_i^2)}\Big)$. Next we use (1.2) to see that the positivity of $\mathrm{Op}\big(\mathrm{e}^{-A}\big)$ is equivalent to $\lambda_i \leq 1$, $i = 1,\dots,d$, which in turn is equivalent to $\sigma(A\theta) \subset [-1,1]$ (the eigenvalues of $A\theta$ are of the form $\pm\lambda_i$). □

Proposition 11. $\mathrm{Sym}_{\mathrm{p}}^{\mathrm{qnd}}(\mathbb{R}^{2d}) = \{A \in \mathrm{Sym}_{++}(\mathbb{R}^{2d}) \mid \sigma(A\theta) \subset]-1,1[\}$.

Proof. We use the basis mentioned at the end of the proof of Proposition 10. □

Proposition 12. $\det(1\!\!1 + A\theta) = \overline{\det(1\!\!1 + \overline{A}\theta)}$. *Consequently,*

$$\mathrm{Sym}^{\mathrm{qnd}}(\mathbb{C}^{2d}) \text{ and } \mathrm{Sym}_{++}^{\mathrm{qnd}}(\mathbb{C}^{2d})$$

are invariant with respect to complex conjugation.

Proof. We use

$$\theta(1\!\!1 + A\theta)\theta = 1\!\!1 + \theta A, \tag{7.3}$$

$$(1\!\!1 + \theta A)^{\#} = 1\!\!1 - A\theta, \tag{7.4}$$

$$\overline{1\!\!1 - A\theta} = 1\!\!1 + \overline{A}\theta. \tag{7.5}$$

□

Theorem 13. (1) *If* $A \in \mathrm{Sym}_{++}(\mathbb{C}^{2d})$, *then* $\overline{A}\#A \in \mathrm{Sym}_{\mathrm{p}}(\mathbb{R}^{2d})$.
(2) *If* $A \in \mathrm{Sym}_{++}^{\mathrm{qnd}}(\mathbb{C}^{2d})$, *then* $\overline{A}\#A \in \mathrm{Sym}_{\mathrm{p}}^{\mathrm{qnd}}(\mathbb{R}^{2d})$.

Proof. (1) Let $A \in \mathrm{Sym}_{++}(\mathbb{C}^{2d})$. Then

$$\mathrm{Op}(\mathrm{e}^{-A})^{*}\mathrm{Op}(\mathrm{e}^{-A}) = \frac{1}{\sqrt{\det(1\!\!1 + \overline{A}\theta A\theta)}}\mathrm{e}^{-\overline{A}\#A} \tag{7.6}$$

is a positive operator. Therefore, by Proposition 10(3), $\overline{A}\#A \in \mathrm{Sym}_{\mathrm{p}}(\mathbb{R}^{2d})$.

(2) $\mathrm{Sym}_{++}^{\mathrm{qnd}}(\mathbb{C}^{2d})$ is a semigroup, invariant with respect to the conjugation, and hence $\overline{A}\#A \in \mathrm{Sym}_{++}^{\mathrm{qnd}}(\mathbb{C}^{2d})$. By (1), $\overline{A}\#A \in \mathrm{Sym}_{\mathrm{p}}(\mathbb{R}^{2d})$. But by definition $\mathrm{Sym}_{\mathrm{p}}^{\mathrm{qnd}}(\mathbb{R}^{2d}) = \mathrm{Sym}_{\mathrm{p}}(\mathbb{R}^{2d}) \cap \mathrm{Sym}_{++}^{\mathrm{qnd}}(\mathbb{C}^{2d})$. □

8. Complex symplectic group

A linear operator R on $\mathbb{R}^{2d}$ is called *symplectic* if

$$R^{\#}\omega R = \omega. \tag{8.1}$$

The set of symplectic operators on $\mathbb{R}^{2d}$ will be denoted $Sp(\mathbb{R}^{2d})$. It is the well known *symplectic group* in dimension $2d$.

In our paper a more important role is played by the complex version of the symplectic group. More precisely, we will say that a complex linear operator R on $\mathbb{C}^{2d}$ is symplectic if (8.1) holds. (Of course, we can replace ω in (8.1) with θ). The set of complex symplectic operators on $\mathbb{C}^{2d}$ will be denoted $Sp(\mathbb{C}^{2d})$. It is also a group, called the *complex symplectic group* in dimension $2d$.

We define

$$Sp_{+}(\mathbb{C}^{2d}) := \{R \in Sp(\mathbb{C}^{2d}) \mid R^{*}\theta R \leq \theta\}, \tag{8.2}$$

$$Sp_{++}(\mathbb{C}^{2d}) := \{R \in Sp(\mathbb{C}^{2d}) \mid R^{*}\theta R < \theta\}. \tag{8.3}$$

Both $Sp_+(\mathbb{C}^{2d})$ and $Sp_{++}(\mathbb{C}^{2d})$ are semigroups satisfying

$$Sp(\mathbb{R}^{2d}) \cap Sp_{++}(\mathbb{C}^{2d}) = \emptyset, \tag{8.4}$$

$$Sp_{++}(\mathbb{C}^{2d}) \subset Sp_+(\mathbb{C}^{2d}), \tag{8.5}$$

$$Sp(\mathbb{R}^{2d}) \subset Sp_+(\mathbb{C}^{2d}). \tag{8.6}$$

We also set

$$Sp_{\mathrm{h}}(\mathbb{C}^{2d}) := \{R \in Sp(\mathbb{C}^{2d}) : \ \overline{R} = R^{-1}\} \tag{8.7}$$

$$= \{R \in Sp(\mathbb{C}^{2d}) : \ R^*\theta = \theta R\}, \tag{8.8}$$

$$Sp_{\mathrm{p}}(\mathbb{C}^{2d}) := \{R \in Sp_{\mathrm{h}}(\mathbb{C}^{2d}) : \ \sigma(R) \subset]0,\infty[\}. \tag{8.9}$$

Below we state a few properties of $Sp_{++}(\mathbb{C}^{2d})$ and $Sp_{\mathrm{p}}(\mathbb{C}^{2d})$. It will be convenient to defer their proofs to the next section.

Proposition 14. $Sp_{\mathrm{p}}(\mathbb{C}^{2d}) \subset Sp_{++}(\mathbb{C}^{2d})$.

Let $t > 0$. Note that $\mathbb{C}\backslash\,]-\infty,0] \ni z \mapsto z^t \in \mathbb{C}$ is a well defined holomorphic function. In the proposition below $\sigma(R) \subset]0,\infty[$, therefore R^t is well defined.

Proposition 15. *Let $R \in Sp_{\mathrm{p}}(\mathbb{C}^{2d})$. Then $R^t \in Sp_{\mathrm{p}}(\mathbb{C}^{2d})$.*

Proposition 16. *Let $R \in Sp_{++}(\mathbb{C}^{2d})$. Then $\overline{R}^{-1}R \in Sp_{\mathrm{p}}(\mathbb{C}^{2d})$.*

The next result, which is an analog of the polar decomposition, was noted by Howe (see [16, Proposition (23.7.2)]):

Proposition 17. *Every $R \in Sp_{++}(\mathbb{C}^{2d})$ may be decomposed in the following way:*

$$R = TS, \tag{8.10}$$

where $T := \overline{R}\sqrt{\overline{R}^{-1}R} \in Sp(\mathbb{R}^{2d})$ and $S := \sqrt{\overline{R}^{-1}R} \in Sp_{\mathrm{p}}(\mathbb{C}^{2d})$.

9. Relationship between Sym and symplectic group

Let us define

$$Sp^{\mathrm{reg}}(\mathbb{C}^{2d}) = \{R \in Sp(\mathbb{C}^{2d}) \mid R + \mathbb{1} \text{ is invertible}\}, \tag{9.1}$$

$$Sp_{\mathrm{h}}^{\mathrm{reg}}(\mathbb{C}^{2d}) = \{R \in Sp_{\mathrm{h}}(\mathbb{C}^{2d}) \mid R + \mathbb{1} \text{ is invertible}\}. \tag{9.2}$$

Theorem 18. (1) $\mathrm{Sym}^{\mathrm{qnd}}(\mathbb{C}^{2d}) \ni A \mapsto c(A\theta) \in Sp^{\mathrm{reg}}(\mathbb{C}^{2d})$ *is a bijection. Its inverse is*

$$Sp^{\mathrm{reg}}(\mathbb{C}^{2d}) \ni R \mapsto c(R)\theta \in \mathrm{Sym}^{\mathrm{qnd}}(\mathbb{C}^{2d}). \tag{9.3}$$

Besides, if $A, B \in \mathrm{Sym}^{\mathrm{qnd}}(\mathbb{C}^{2d})$ and $A\#B \in \mathrm{Sym}^{\mathrm{qnd}}(\mathbb{C}^{2d})$ is well defined, then

$$c(A\#B\theta) = c(A\theta)c(B\theta). \tag{9.4}$$

(2) $\mathrm{Sym}^{\mathrm{qnd}}_{++}(\mathbb{C}^{2d}) \ni A \mapsto c(A\theta) \in Sp_{++}(\mathbb{C}^{2d})$ *is an isomorphism of semigroups.*

(3) $\mathrm{Sym}^{\mathrm{qnd}}(\mathbb{R}^{2d}) \ni A \mapsto c(A\theta) \in Sp_{\mathrm{h}}^{\mathrm{reg}}(\mathbb{C}^{2d})$ *is a bijection.*

(4) $\mathrm{Sym}_{\mathrm{p}}^{\mathrm{qnd}}\big(\mathbb{R}^{2d}\big) \ni A \mapsto c(A\theta) \in Sp_{\mathrm{p}}\big(\mathbb{C}^{2d}\big)$ *is a bijection.*

Proof. (1) Let $A \in \mathrm{Sym}^{\mathrm{qnd}}\big(\mathbb{C}^{2d}\big)$. Then,

$$\begin{aligned} c(A\theta)^{\#}\theta c(A\theta) &= (\mathbb{1}-\theta A)^{-1}(\mathbb{1}+\theta A)\theta(\mathbb{1}-A\theta)(\mathbb{1}+A\theta)^{-1} \\ &= (\mathbb{1}-\theta A)^{-1}(\mathbb{1}-\theta A\theta A\theta)(\mathbb{1}+A\theta)^{-1} \\ &= (\mathbb{1}-\theta A)^{-1}(\mathbb{1}-\theta A)\theta(\mathbb{1}+A\theta)(\mathbb{1}+A\theta)^{-1} \;=\; \theta. \end{aligned}$$

Hence, $c(A\theta) \in Sp\big(\mathbb{C}^{2d}\big)$.

Conversely, let $R \in Sp^{\mathrm{reg}}\big(\mathbb{C}^{2d}\big)$. Then

$$\begin{aligned} \Big((\mathbb{1}-R)(\mathbb{1}+R)^{-1}\theta\Big)^{\#} &= -\theta(\mathbb{1}+R^{\#})^{-1}(\mathbb{1}-R^{\#}) \\ &= -(\theta+R^{\#}\theta)^{-1}(\mathbb{1}-R^{\#}) = -\big(\theta(\mathbb{1}+R^{-1})\big)^{-1}(\mathbb{1}-R^{\#}) \\ &= -(\mathbb{1}+R^{-1})^{-1}(\theta-\theta R^{\#}) = -(\mathbb{1}+R^{-1})^{-1}(\mathbb{1}-R^{-1})\theta \\ &= (\mathbb{1}+R)^{-1}(\mathbb{1}-R)\theta. \end{aligned}$$

Hence, $c(R)\theta \in \mathrm{Sym}\big(\mathbb{C}^{2d}\big)$.

Clearly, $A\theta + \mathbb{1}$ is invertible iff $c(A\theta) \in L^{\mathrm{reg}}\big(\mathbb{C}^{2d}\big)$. Thus

$$\mathrm{Sym}^{\mathrm{qnd}}\big(\mathbb{C}^{2d}\big) \ni A \mapsto c(A\theta) \in Sp^{\mathrm{reg}}\big(\mathbb{C}^{2d}\big)$$

is a bijection.

To see (9.4) it is enough to use (5.5).

(2) We have

$$\begin{aligned} c(A\theta)^{*}\theta c(A\theta) &= (\mathbb{1}+\theta\overline{A})^{-1}(\mathbb{1}-\theta\overline{A})\theta(\mathbb{1}-A\theta)(\mathbb{1}+A\theta)^{-1} \\ &= (\mathbb{1}+\theta\overline{A})^{-1}(\mathbb{1}-\theta\overline{A}\theta-\theta A\theta+\theta\overline{A}\theta A\theta)(\mathbb{1}+A\theta)^{-1} \\ &= \theta - 2(\mathbb{1}+\theta\overline{A})^{-1}\theta(\overline{A}+A)\theta(\mathbb{1}+A\theta)^{-1}. \end{aligned}$$

Thus,

$$c(A\theta)^{*}\theta c(A\theta) < \theta \tag{9.5}$$

iff $\overline{A} + A > 0$. Hence $\mathrm{Sym}_{++}^{\mathrm{qnd}}\big(\mathbb{C}^{2d}\big) \ni A \mapsto c(A\theta) \in Sp_{++}\big(\mathbb{C}^{2d}\big)$ is a bijection. It is a homomorphism because of (9.4).

(3) Let $A \in \mathrm{Sym}^{\mathrm{qnd}}\big(\mathbb{R}^{2d}\big)$. Then

$$\overline{c(A\theta)} = \frac{\mathbb{1}+A\theta}{\mathbb{1}-A\theta} = c(A\theta)^{-1}. \tag{9.6}$$

Hence, $c(A\theta) \in Sp_{\mathrm{h}}\big(\mathbb{C}^{2d}\big)$.

Conversely, let $R \in Sp_{\mathrm{h}}^{\mathrm{reg}}\big(\mathbb{C}^{2d}\big)$. Then

$$\overline{(\mathbb{1}-R)(\mathbb{1}+R)^{-1}\theta} \;=\; -(\mathbb{1}-\overline{R})(\mathbb{1}+\overline{R})^{-1}\theta \tag{9.7}$$

$$= -(\mathbb{1}-R^{-1})(\mathbb{1}+R^{-1})^{-1}\theta \;=\; (\mathbb{1}-R)(\mathbb{1}+R)^{-1}\theta. \tag{9.8}$$

Hence, $c(R)\theta \in \mathrm{Sym}\big(\mathbb{R}^{2d}\big)$.

(4) Clearly,

$$\lambda \in]-1,1[\quad \text{iff} \quad \frac{1-\lambda}{1+\lambda} \in]0,\infty[.$$

Therefore,

$$\sigma(A\theta) \subset]-1,1[\quad \text{iff} \quad \sigma\big(c(A\theta)\big) \subset]0,\infty[.$$

Then we use the characterization of $\mathrm{Sym}_{\mathrm{p}}^{\mathrm{qnd}}\big(\mathbb{R}^{2d}\big)$ given in Proposition 11. □

Proof of Proposition 14. Let $R \in Sp_{\mathrm{p}}\big(\mathbb{C}^{2d}\big)$. By Theorem 18(4),

$$c(R)\theta \in \mathrm{Sym}_{\mathrm{p}}^{\mathrm{qnd}}\big(\mathbb{R}^{2d}\big).$$

Proposition 11 implies that $c(R)\theta \in \mathrm{Sym}_{++}^{\mathrm{qnd}}\big(\mathbb{R}^{2d}\big)$. Now Theorem 18(2) shows that $R = c\big((c(R)\theta)\theta\big) \in Sp_{++}\big(\mathbb{C}^{2d}\big)$. □

Proof of Proposition 15. Let $R \in Sp_{\mathrm{p}}\big(\mathbb{C}^{2d}\big)$.

Functional calculus of operators is invariant with respect to similarity transformations. Therefore, $R^{\#(-1)} = \theta R \theta^{-1}$ implies $R^{\#(-t)} = \theta R^t \theta^{-1}$. Hence $R^t \in Sp\big(\mathbb{C}^{2d}\big)$.

$\overline{R} = R^{-1}$ implies $\overline{R}^t = (R^t)^{-1}$. Hence, $R^t \in Sp_{\mathrm{h}}\big(\mathbb{C}^{2d}\big)$.

$\sigma(R) \subset]0,\infty[$ implies $\sigma(R^t) \subset]0,\infty[$. Hence $R^t \in Sp_{\mathrm{p}}\big(\mathbb{C}^{2d}\big)$. □

Proof of Proposition 16. Theorem 18(2) assures us that we can find a matrix $A \in \mathrm{Sym}_{++}^{\mathrm{qnd}}\big(\mathbb{R}^{2d}\big)$, such that $c(A\theta) = R$. By Theorem 13(2), $\overline{A} \# A \in \mathrm{Sym}_{\mathrm{p}}^{\mathrm{qnd}}\big(\mathbb{R}^{2d}\big)$. Now we may use Theorem 18(4) to see that $c(\overline{A}\#A\theta) \in Sp_{\mathrm{p}}\big(\mathbb{C}^{2d}\big)$.

It is easy to check that $\overline{R}^{-1} = c(\overline{A}\theta)$. Moreover, by (9.4),

$$\overline{R}^{-1} R = c\big(\overline{A}\theta\big) c(A\theta) = c\big(\overline{A}\#A\theta\big). \tag{9.9}$$

Therefore, $\overline{R}^{-1} R \in Sp_{\mathrm{p}}\big(\mathbb{C}^{2d}\big)$. □

Proof of Proposition 17. By Proposition 16, we have $\overline{R}^{-1} R \in Sp_{\mathrm{p}}\big(\mathbb{C}^{2d}\big)$, while Proposition 15 yields $S := \sqrt{\overline{R}^{-1} R} \in Sp_{\mathrm{p}}\big(\mathbb{C}^{2d}\big)$. Clearly, $\overline{R} \in Sp\big(\mathbb{C}^{2d}\big)$. Hence, $T := \overline{R}S \in Sp\big(\mathbb{C}^{2d}\big)$.

$$\overline{T} = \overline{\overline{R}S} = RS^{-1} = RS^{-2}S = R\,R^{-1}\overline{R}\,S = T. \tag{9.10}$$

Therefore, $T := \overline{R}S \in Sp\big(\mathbb{R}^{2d}\big)$. □

Theorem 19. *The map*

$$\mathrm{Osc}_{++}^{\mathrm{nor}}\big(\mathbb{C}^{2d}\big) \ni \pm\sqrt{\det(\mathbb{1} + A\theta)}\mathrm{Op}\big(\mathrm{e}^{-A}\big) \mapsto c(A\theta) \in Sp_{++}\big(\mathbb{C}^{2d}\big)$$

is a 2–1 epimorphism of semigroups.

Proof. We use Proposition 9 and Theorem 18(2). □

10. Metaplectic group

It is easy to see that if $C \in \mathrm{Sym}\big(\mathbb{R}^{2d}\big)$, then $c(C\omega) \in Sp\big(\mathbb{R}^{2d}\big)$. In fact, elements of this form constitute an open dense subset of $Sp\big(\mathbb{R}^{2d}\big)$.

We define $Mp(\mathbb{R}^{2d})$, called the metaplectic group in dimension $2d$, to be the group generated by operators of the form

$$\pm\sqrt{\det(\mathbb{1} + C\omega)}\mathrm{Op}\big(\mathrm{e}^{-\mathrm{i}C}\big), \quad C \in \mathrm{Sym}\big(\mathbb{R}^{2d}\big). \tag{10.1}$$

The theory of the metaplectic group is well known, see, e.g., [11, Sect. 10.3.1]. We assume that the reader is familiar with its basic elements. Actually, we have already used it in our proof of Proposition 10(3).

The theory of the metaplectic group can be summed up by the following theorem:

Theorem 20. *The metaplectic group consists of unitary operators. Operators of the form* (10.1) *constitute an open and dense subset of* $Mp(\mathbb{R}^{2d})$*. The map*

$$\pm\sqrt{\det(\mathbb{1} + C\omega)}\mathrm{Op}\big(\mathrm{e}^{-\mathrm{i}C}\big) \mapsto c(C\omega) \tag{10.2}$$

extends by continuity to a 2–1 *epimorphism* $Mp\big(\mathbb{R}^{2d}\big) \to Sp\big(\mathbb{R}^{2d}\big)$

Remark 1. For completeness, one should mention some other natural semigroups closely related to $\mathrm{Osc}_{++}\big(\mathbb{C}^{2d}\big)$:

1. $\mathrm{Osc}_{+}\big(\mathbb{C}^{2d}\big)$ generated by operators $a\mathrm{Op}(\mathrm{e}^{-A})$ with $A \in \mathrm{Sym}_{+}\big(\mathbb{C}^{2d}\big)$, $a \in \mathbb{C}$;
2. $\mathrm{Osc}_{+}^{\mathrm{nor}}\big(\mathbb{C}^{2d}\big)$ generated by operators of the form $\pm\sqrt{\det(\mathbb{1} + A\theta)}\mathrm{Op}\big(\mathrm{e}^{-A}\big)$ with $A \in \mathrm{Sym}_{+}\big(\mathbb{C}^{2d}\big)$.

11. Polar decomposition

For an operator V, its *absolute value* is defined as

$$|V| := \sqrt{V^*V}. \tag{11.1}$$

The following theorem provides a formula for the absolute value of elements of the oscillator semigroup.

Theorem 21. *Let* $A \in \mathrm{Sym}_{++}^{\mathrm{qnd}}\big(\mathbb{C}^{2d}\big)$*. Then*

$$\big|\mathrm{Op}(\mathrm{e}^{-A})\big| = \frac{\sqrt[4]{\det\big(\mathbb{1} + (B\theta)^2\big)}}{\sqrt[4]{\det(\mathbb{1} + \overline{A}\theta A\theta)}}\mathrm{Op}\big(\mathrm{e}^{-B}\big), \tag{11.2}$$

where

$$B = c\Big(\sqrt{c(\overline{A}\theta)c(A\theta)}\Big)\theta. \tag{11.3}$$

Besides, the function

$$\mathrm{Sym}_{++}^{\mathrm{qnd}}\big(\mathbb{C}^{2d}\big) \ni A \mapsto \big|\mathrm{Op}\big(\mathrm{e}^{-A}\big)\big|$$

is smooth.

Proof. By Proposition 16, $c(\overline{A}\theta)c(A\theta) = \overline{c(A\theta)}^{-1}c(A\theta) \in Sp_{\mathrm{p}}\big(\mathbb{C}^{2d}\big)$. Hence, by Proposition 15, we can define $\sqrt{c(\overline{A}\theta)c(A\theta)} \in Sp_{\mathrm{p}}\big(\mathbb{C}^{2d}\big)$. Therefore, B defined in (11.3) belongs to $\mathrm{Sym}_{\mathrm{p}}^{\mathrm{qnd}}\big(\mathbb{R}^{2d}\big)$ and satisfies $\overline{A}\#A = B\#B$.

We have

$$\mathrm{Op}\big(\mathrm{e}^{-B}\big)^2 = \frac{1}{\sqrt{\det(\mathbb{1} + (B\theta)^2}}\mathrm{Op}\big(\mathrm{e}^{-B\#B}\big). \tag{11.4}$$

Hence,

$$\mathrm{Op}\big(\mathrm{e}^{-A}\big)^*\mathrm{Op}\big(\mathrm{e}^{-A}\big) \quad = \quad \frac{\sqrt{\det\big(\mathbb{1} + (B\theta)^2\big)}}{\sqrt{\det(\mathbb{1} + \overline{A}\theta A\theta)}}\mathrm{Op}\big(\mathrm{e}^{-B}\big)^2. \tag{11.5}$$

Besides, $\mathrm{Op}\big(\mathrm{e}^{-B}\big) \geq 0$. Therefore, $\big|\mathrm{Op}\big(\mathrm{e}^{-A}\big)\big|$ is given by (11.2).

Now the square root is a smooth function on the set of invertible matrices (and obviously on the set of nonzero numbers). In the formula (11.3) for $A \in \mathrm{Sym}_{++}^{\mathrm{qnd}}\big(\mathbb{C}^{2d}\big)$, we never need to take roots of zero or of non-invertible matrices, because $\mathbb{1} \pm A\theta$ and $\mathbb{1} \pm \overline{A}\theta$ are invertible. Therefore,

$$\mathrm{Sym}_{++}^{\mathrm{qnd}}\big(\mathbb{C}^{2d}\big) \ni A \mapsto \sqrt{c(\overline{A}\theta)c(A\theta)} \tag{11.6}$$

is smooth. Therefore, the map $A \mapsto B$ is smooth

For $A \in \mathrm{Sym}_{++}^{\mathrm{qnd}}\big(\mathbb{C}^{2d}\big)$, $\overline{A}, B \in \mathrm{Sym}_{++}^{\mathrm{qnd}}\big(\mathbb{C}^{2d}\big)$. Therefore, by Proposition 5.10, $\mathbb{1}+\overline{A}\theta A\theta$ and $\mathbb{1}+(B\theta)^2$ are invertible. Hence, the prefactors of (11.2) are smooth. This ends the proof of the smoothness of (11.2). $\square$

Let V be a closed operator such that $\mathrm{Ker}V = \mathrm{Ker}V^* = \{0\}$. Then it is well known that there exists a unique unitary operator U such that we have the identity

$$V = U|V|. \tag{11.7}$$

called the *polar decomposition*.

Theorem 22. *Let* $A \in \mathrm{Sym}_{++}^{\mathrm{qnd}}\big(\mathbb{C}^{2d}\big)$. *Let* $B \in \mathrm{Sym}_{\mathrm{p}}^{\mathrm{qnd}}\big(\mathbb{C}^{2d}\big)$ *be defined as in* (11.3). *Then*

$$\Big|\sqrt{\det(\mathbb{1} + A\theta)}\mathrm{Op}\big(\mathrm{e}^{-A}\big)\Big| = \sqrt{\det(\mathbb{1} + B\theta)}\mathrm{Op}\big(\mathrm{e}^{-B}\big), \tag{11.8}$$

and the unitary operator U *that appears in the polar decomposition*

$$\sqrt{\det(\mathbb{1} + A\theta)}\mathrm{Op}\big(\mathrm{e}^{-A}\big) = U\sqrt{\det(\mathbb{1} + B\theta)}\mathrm{Op}\big(\mathrm{e}^{-B}\big) \tag{11.9}$$

belongs to $Mp\big(\mathbb{R}^{2d}\big)$. *Besides, if*

$$\mathrm{i}C := A\#(-B) \tag{11.10}$$

is well defined, then

$$U = \epsilon\sqrt{\det(\mathbb{1} + C\omega)}\mathrm{Op}\big(\mathrm{e}^{-\mathrm{i}C}\big), \tag{11.11}$$

where $\epsilon = 1$ *or* $\epsilon = -1$.

Proof. By (5.10),

$$\mathbb{1} + \overline{A}\theta A\theta = (\mathbb{1} + \overline{A}\theta)(\mathbb{1} + \overline{A}\#A\theta)^{-1}(\mathbb{1} + A\theta), \tag{11.12}$$

$$\mathbb{1} + B\theta B\theta = (\mathbb{1} + B\theta)(\mathbb{1} + B\#B\theta)^{-1}(\mathbb{1} + B\theta), \tag{11.13}$$

Besides, $\overline{A}\#A = B\#B$. This together with (11.2) implies (11.8).

Assume now that $\mathrm{i}C := A\#(-B)$ is well defined. Then clearly

$$\begin{aligned}&\sqrt{\det(\mathbb{1} + A\theta)}\operatorname{Op}\big(\mathrm{e}^{-A}\big)\\ &= \epsilon\sqrt{\det(\mathbb{1} + B\theta)}\operatorname{Op}\big(\mathrm{e}^{-B}\big)\sqrt{\det(\mathbb{1} + \mathrm{i}C\theta)}\operatorname{Op}\big(\mathrm{e}^{-\mathrm{i}C}\big).\end{aligned} \tag{11.14}$$

It remains to show that $\mathrm{i}C$ is purely imaginary.

$$\overline{A\#(-B)} = (-B)\#\overline{A} = (-B)\#\overline{A}\#A(-A) \tag{11.15}$$

$$= (-B)\#B\#B\#(-A) \tag{11.16}$$

$$= B\#(-A) = -A\#(-B). \tag{11.17}$$

□

12. Trace and the trace norm

Suppose we have an operator K on $\mathrm{L}^2\big(\mathbb{R}^d\big)$. As proven in [13] (for a more general setting, see [4, 5]), if K has a continuous kernel $K(x,\, y)$ belonging to $\mathrm{L}^2\big(\mathbb{R}^d \times \mathbb{R}^d\big)$ and $x \mapsto K(x,\, x)$ is in $\mathrm{L}^1\big(\mathbb{R}^d\big)$, then

$$\operatorname{Tr} K = \int K(x,\, x)\,\mathrm{d}x. \tag{12.1}$$

In the case of Weyl–Wigner quantization, for a symbol k we get

$$\operatorname{Tr}\operatorname{Op}(k) = \int \operatorname{Op}(k)(x,\, x)\,\mathrm{d}x = (2\pi)^{-d}\int k(x,\, \xi)\,\mathrm{d}x\,\mathrm{d}\xi. \tag{12.2}$$

This easily implies the following proposition:

Proposition 23. *The trace of operator* $\operatorname{Op}\big(\mathrm{e}^{-A}\big)$ *with* $A \in \mathrm{Sym}_{++}\big(\mathbb{C}^{2d}\big)$ *is*

$$\operatorname{Tr}\operatorname{Op}\big(\mathrm{e}^{-A}\big) = \frac{1}{2^d\sqrt{\det A}} = \frac{1}{2^d\sqrt{\det A\theta}}. \tag{12.3}$$

(Note that $\det\theta = 1$, hence we could insert θ in (12.3)).

One can also compute the trace of the absolute value of elements of the oscillator semigroup, the so-called trace norm.

Theorem 24. *The trace norm of* $\operatorname{Op}\big(\mathrm{e}^{-A}\big)$, *where* $A \in \mathrm{Sym}_{++}\big(\mathbb{C}^{2d}\big)$, *is*

$$\operatorname{Tr}\big|\operatorname{Op}\big(\mathrm{e}^{-A}\big)\big| = \frac{\sqrt{2}}{2^d\sqrt{\det\big|(\mathbb{1} + A\theta)\big(\mathbb{1} - \sqrt{c(A^*\theta)c(A\theta)}\big)\big|}}. \tag{12.4}$$

Proof. Equations (12.3) and (11.2) imply

$$\operatorname{Tr}\big|\operatorname{Op}\big(\mathrm{e}^{-A}\big)\big| = \frac{\sqrt[4]{\det\big(\mathbb{1}+(B\theta)^2\big)}}{2^d\sqrt[4]{\det(\mathbb{1}+\overline{A}\theta A\theta)(B\theta)^2}}. \tag{12.5}$$

Now, easy algebra shows that

$$\begin{aligned}\frac{\det\big(\mathbb{1}+(B\theta)^2\big)}{\det(\mathbb{1}+\overline{A}\theta A\theta)(B\theta)^2} &= \frac{2\det\big(\mathbb{1}+c(\overline{A}\theta)c(A\theta)\big)}{\det(\mathbb{1}+\overline{A}\theta A\theta)\big(\mathbb{1}-\sqrt{c(\overline{A}\theta)c(A\theta)}\big)^2}\\ &= \frac{4}{\det(\mathbb{1}+\overline{A}\theta)(\mathbb{1}+A\theta)\big(\mathbb{1}-\sqrt{c(\overline{A}\theta)c(A\theta)}\big)^2}\\ &= \frac{2^2}{\Big(\det\Big|(\mathbb{1}+A\theta)\Big(\mathbb{1}-\sqrt{c(\overline{A}\theta)c(A\theta)}\Big)\Big|\Big)^2}.\end{aligned}$$

□

Corollary 25. *The trace norm of* $\operatorname{Op}\big(\mathrm{e}^{-B}\big)$, *where* $B\in\operatorname{Sym}_{++}\big(\mathbb{R}^{2d}\big)$, *is*

$$\operatorname{Tr}\big|\operatorname{Op}\big(\mathrm{e}^{-B}\big)\big| = \frac{\sqrt{2}}{2^d\sqrt{\det\big||\mathbb{1}+B\theta|-|\mathbb{1}-B\theta|\big|}}. \tag{12.6}$$

Thus, if we diagonalize simultaneously B and ω, as in the proof of Proposition 10, then

$$\operatorname{Tr}\big|\operatorname{Op}\big(\mathrm{e}^{-B}\big)\big| = \frac{\sqrt{2}}{4^d\prod\limits_{\lambda_i<1}\lambda_i}. \tag{12.7}$$

13. Operator norm

Proposition 26. *Let* $B\in\operatorname{Sym}_{++}\big(\mathbb{R}^{2d}\big)$. *Then*

$$\big\|\operatorname{Op}\big(\mathrm{e}^{-B}\big)\big\| = \frac{1}{\sqrt{\det(\mathbb{1}+\sqrt{B\theta B\theta})}}. \tag{13.1}$$

Proof. First, using (1.2), we check that in the case of one degree of freedom we have

$$\Big\|\operatorname{Op}\Big(\mathrm{e}^{-\lambda(x^2+p^2)}\Big)\Big\| = \frac{1}{1+\lambda}. \tag{13.2}$$

An arbitrary B we can diagonalize together with θ, as in the proof of Proposition 10(3), and then we obtain

$$\big\|\operatorname{Op}\big(\mathrm{e}^{-B}\big)\big\| = \prod_{i=1}^{d}\frac{1}{1+\lambda_i}. \tag{13.3}$$

Now the right-hand side of (13.3) can be rewritten as the right-hand side of (13.1). □

Using (11.8), we obtain an identity for an arbitrary element of the oscillator semigroup. A closely related result is described in [21, Theorem 5.2].

Theorem 27. *Let* $A \in \mathrm{Sym}_{++}(\mathbb{C}^{2d})$. *Then*

$$\begin{aligned}&\left\|\sqrt{\det(\mathbb{1}+A\theta)}\mathrm{Op}(\mathrm{e}^{-A})\right\|\\ &\qquad = \frac{\sqrt{\det\left(\mathbb{1}+c\left(\sqrt{c(\overline{A}\theta)c(A\theta)}\right)\right)}}{\sqrt{\det\left(\mathbb{1}+\sqrt{c\left(\sqrt{c(\overline{A}\theta)c(A\theta)}\right)c\left(\sqrt{c(\overline{A}\theta)c(A\theta)}\right)}\right)}}.\end{aligned} \tag{13.4}$$

14. One degree of freedom

In the case of one degree of freedom we have a complete characterization of quantum nondegenerate symmetric matrices.

Theorem 28. *Let* $A \in \mathrm{Sym}(\mathbb{C}^2)$. *Then* $A \in \mathrm{Sym}^{\mathrm{qnd}}(\mathbb{C}^2)$ *iff* $\det A \neq 1$.

Proof. We easily compute that for $A \in \mathrm{Sym}(\mathbb{C}^2)$,

$$\det(\mathbb{1}+A\theta) = 1-\det A. \qquad \square$$

Next we describe the quantum degenerate case for one degree of freedom on the level of the oscillator group.

Theorem 29. *Elements of* $\mathrm{Osc}_{++}(\mathbb{C}^2)$ *that are not proportional to an element of* $\mathrm{Osc}_{++}^{\mathrm{nor}}(\mathbb{C}^2)$ *are proportional to a projection. They have the integral kernel of the form*

$$c\mathrm{e}^{-(ax^2+by^2)}, \tag{14.1}$$

where $a,b,c \in \mathbb{C}$, $\mathrm{Re}\,a, \mathrm{Re}\,b > 0$. *The Weyl symbol of the operator with the kernel* (14.1) *is*

$$c\frac{2\sqrt{\pi}}{\sqrt{a+b}}\mathrm{e}^{-A}, \tag{14.2}$$

where

$$A = \frac{1}{(a+b)}\begin{bmatrix} 4ab & \mathrm{i}(-a+b) \\ \mathrm{i}(-a+b) & 1 \end{bmatrix}. \tag{14.3}$$

Matrices of the form (14.3) *with* $\mathrm{Re}\,a, \mathrm{Re}\,b > 0$ *are precisely all matrices in*

$$\mathrm{Sym}_{++}(\mathbb{C}^2)\backslash\mathrm{Sym}_{++}^{\mathrm{qnd}}(\mathbb{C}^2). \tag{14.4}$$

15. Application to the boundedness of pseudo-differential operators

Cordes proved the following result [10]:

Theorem 30. *Suppose* $k \in \mathscr{S}'\big(\mathbb{R}^d \times \mathbb{R}^d\big)$ *and* $s > \frac{d}{2}$*. Then there exists a constant* $c_{d,s}$ *such that*

$$\|\mathrm{Op}(k)\| \leqslant c_{d,s}\|(1-\Delta_x)^s(1-\Delta_p)^s k\|_\infty. \tag{15.1}$$

The above result can be called the *Calderón and Vaillancourt Theorem for the Weyl quantization*. (The original result of Calderón and Vaillancourt [9] concerned the $x-p$ quantization, known also as the standard or Kohn–Nirenberg quantization).

Note that Theorem 30 is not optimal with respect to the number of derivatives. The optimal bound on the number of derivatives for the Weyl quantization is $s > \frac{d}{4}$. It was discovered by A. Boulkhemair [3] and it requires a different proof than the one developed by Cordes.

In what follows we will describe a proof of Theorem 30 which gives an estimate of $c_{d,s}$. We will follow the ideas of Cordes and Kato ([10] and [18]), who however do not give an explicit bound on the constant $c_{d,s}$. The estimate (1.4) for the trace norm of operators with Gaussian symbols plays an important role in our proof.

We start with the following proposition.

Proposition 31. *For* $s > \frac{d}{2}$*, define the functions*

$$\psi_s(\xi) := (2\pi)^{-d}\int \mathrm{d}\zeta\,(1+\zeta^2)^{-s}\mathrm{e}^{\mathrm{i}\zeta\xi}, \tag{15.2}$$

$$P_s(x,p) := \psi_s(x)\psi_s(p). \tag{15.3}$$

Then $\mathrm{Op}(P_s)$ *is of trace class and*

$$\mathrm{Tr}\left|\mathrm{Op}(P_s)\right| \leq \frac{\Gamma(s)^2 + \Gamma(s-\frac{d}{2})^2}{(2\pi)^d\Gamma(s)^2}. \tag{15.4}$$

Proof. Let us use the so-called Schwinger parametrization

$$X^{-s} = \frac{1}{\Gamma(s)}\int_0^\infty \mathrm{e}^{-tX}t^{s-1}\,\mathrm{d}t \tag{15.5}$$

to get

$$\begin{aligned}\psi_s(\xi) &= \frac{1}{\Gamma(s)(2\pi)^d}\int_0^\infty \mathrm{d}t\int \mathrm{d}\zeta\,\mathrm{e}^{-t(1+\zeta^2)}t^{s-1}\mathrm{e}^{\mathrm{i}\zeta\xi}\\ &= \frac{1}{\pi^{\frac{d}{2}}2^d\Gamma(s)}\int_0^\infty \mathrm{d}t\,t^{s-\frac{d}{2}-1}\mathrm{e}^{-t-\frac{\xi^2}{4t}}.\end{aligned} \tag{15.6}$$

Now

$$P_s(x,p) = \frac{1}{\pi^d 2^{2d}\Gamma^2(s)} \int_0^\infty \mathrm{d}u \int_0^\infty \mathrm{d}v \mathrm{e}^{-u-v-\frac{x^2}{4u}-\frac{p^2}{4v}} (uv)^{s-\frac{d}{2}-1}. \tag{15.7}$$

By (1.4), we have

$$\mathrm{Tr}\left|\mathrm{Op}\big(\mathrm{e}^{-\alpha x^2-\beta p^2}\big)\right| = \begin{cases} \frac{1}{(2\sqrt{\alpha\beta})^d}, & \alpha\beta \le 1, \\ \frac{1}{2^d}, & 1 \le \alpha\beta. \end{cases} \tag{15.8}$$

Hence,

$$\begin{aligned} &\mathrm{Tr}\left|\mathrm{Op}(P_s)\right| \\ &\le \frac{1}{2^{2d}\pi^d\Gamma^2(s)} \int_0^\infty \mathrm{d}u \int_0^\infty \mathrm{d}v \mathrm{e}^{-u-v} \mathrm{Tr}\left|\mathrm{Op}\Big(\mathrm{e}^{-\frac{x^2}{4u}-\frac{p^2}{4v}}\Big)\right| (uv)^{s-\frac{d}{2}-1} \\ &\le \frac{1}{2^d\pi^d\Gamma^2(s)} \Bigg(\underset{4\le uv,\ u,v>0}{\int \mathrm{d}u \int \mathrm{d}v}\ \mathrm{e}^{-u-v}(uv)^{s-1} + \underset{uv\le 4,\ u,v>0}{\int \mathrm{d}u \int \mathrm{d}v}\ \mathrm{e}^{-u-v}(uv)^{s-\frac{d}{2}-1} \Bigg) \\ &\le \frac{\Gamma(s)^2 + \Gamma(s-\frac{d}{2})^2}{2^d\pi^d\Gamma^2(s)}. \end{aligned} \tag{15.9}$$

□

Proposition 32. *Let B be a self-adjoint trace class operator and $h \in L^\infty(\mathbb{R}^{2d})$. Then*

$$C := \frac{1}{(2\pi)^d} \int \mathrm{d}y \int \mathrm{d}w h(y,w) \mathrm{e}^{-\mathrm{i}y\hat{p}+\mathrm{i}w\hat{x}} B \mathrm{e}^{\mathrm{i}y\hat{p}-\mathrm{i}w\hat{x}} \tag{15.10}$$

is bounded and

$$\|C\| \le \mathrm{Tr}\,|B|\,\|h\|_\infty. \tag{15.11}$$

Proof. For $\Phi \in L^2\big(\mathbb{R}^d\big)$, $\|\Phi\| = 1$, define $T_\Phi : L^2\big(\mathbb{R}^d\big) \to L^2\big(\mathbb{R}^{2d}\big)$ by

$$T_\Phi\Theta(y,w) := (2\pi)^{-\frac{d}{2}} \big(\Phi|\mathrm{e}^{\mathrm{i}y\hat{p}-\mathrm{i}w\hat{x}}\Theta\big), \quad \Theta \in L^2\big(\mathbb{R}^{2d}\big). \tag{15.12}$$

We check that T_Φ is an isometry. This implies that for $\Phi, \Psi \in L^2\big(\mathbb{R}^d\big)$ of norm one

$$\frac{1}{(2\pi)^d} \int \mathrm{d}y \int \mathrm{d}w h(y,w) \mathrm{e}^{-\mathrm{i}y\hat{p}+\mathrm{i}w\hat{x}} |\Phi)(\Psi| \mathrm{e}^{\mathrm{i}y\hat{p}-\mathrm{i}w\hat{x}} \tag{15.13}$$

is bounded and its norm is less than $\|h\|_\infty$. Indeed, (15.13) can be written as the product of three operators

$$T_\Phi^* h T_\Psi, \tag{15.14}$$

where h is meant to be the operator of the multiplication by the function h on the space $L^2(\mathbb{R}^{2d})$. Now it suffices to write

$$B = \sum_{i=1}^\infty \lambda_i |\Phi_i)(\Psi_i|, \tag{15.15}$$

where Φ_i, Ψ_i are normalized, $\lambda_i \geq 0$ and $\operatorname{Tr}|B| = \sum_{i=1}^{\infty} \lambda_i$. □

Proof of Theorem 30. Set

$$h := (1 - \Delta_x)^s (1 - \Delta_p)^s k. \tag{15.16}$$

Then

$$\begin{aligned} k(x,p) &= (1-\Delta_x)^{-s}(1-\Delta_p)^{-s} h(x,p) \\ &= \int \mathrm{d}y \int \mathrm{d}w \, P_s(x-y, p-w) h(y,w). \end{aligned} \tag{15.17}$$

Hence

$$\begin{aligned} \operatorname{Op}(k) &= \int \mathrm{d}y \int \mathrm{d}w \operatorname{Op}\big(P_s(x-y,p-w)\big) h(y,w) \\ &= \frac{1}{(2\pi)^d} \int \mathrm{d}y \int \mathrm{d}w \, h(y,w) \mathrm{e}^{-\mathrm{i}y\hat{p} + \mathrm{i}w\hat{x}} \operatorname{Op}(P_s) \mathrm{e}^{\mathrm{i}y\hat{p} - \mathrm{i}w\hat{x}}. \end{aligned} \tag{15.18}$$

Therefore, by Proposition 32,

$$\|\operatorname{Op}(k)\| \leq \operatorname{Tr}\big|\operatorname{Op}(P_s)\big| \|h\|_\infty. \tag{15.19}$$

Thus we can set

$$c_{d,s} = \operatorname{Tr}\big|\operatorname{Op}(P_s)\big|, \tag{15.20}$$

which is finite by Proposition 31. □

Proposition 31 yields an explicit estimate for $c_{d,s}$ given by the right-hand side of (15.4). Actually, in the proof of Proposition 31 we have an even better, although more complicated explicit estimate given by (15.9).

16. Complex symplectic Lie algebra

The well known *symplectic Lie algebra* in dimension $2d$ is defined as the set of $R \in L(\mathbb{R}^{2d})$ satisfying

$$R^{\#}\omega + \omega R = 0. \tag{16.1}$$

Similarly, the set of $R \in L(\mathbb{C}^{2d})$ satisfying (16.1) is called the *complex symplectic Lie algebra* in dimension $2d$ and denoted $sp(\mathbb{C}^{2d})$. As usual in the complex case, we usually prefer to replace ω in (16.1) with θ.

We define

$$sp_+(\mathbb{C}^{2d}) := \{D \in sp(\mathbb{C}^{2d}) \mid D^*\theta + \theta D \geq 0\}, \tag{16.2}$$

$$sp_{++}(\mathbb{C}^{2d}) := \{D \in sp(\mathbb{C}^{2d}) \mid D^*\theta + \theta D > 0\}. \tag{16.3}$$

We also introduce

$$sp_{\mathrm{h}}(\mathbb{C}^{2d}) := \{D \in sp(\mathbb{C}^{2d}) \mid \overline{D} = -D\}, \tag{16.4}$$

$$sp_{\mathrm{p}}(\mathbb{C}^{2d}) := \{D \in sp_{\mathrm{h}}(\mathbb{C}^{2d}) \mid \theta D > 0\}. \tag{16.5}$$

Proposition 33. (1) *Let* $D \in sp(\mathbb{C}^{2d})$. *Then* $\mathrm{e}^{-D} \in Sp(\mathbb{C}^{2d})$.
(2) *Let* $D \in sp_{++}(\mathbb{C}^{2d})$. *Then* $\mathrm{e}^{-D} \in Sp_{++}(\mathbb{C}^{2d})$.

(3) *Let* $D \in sp_{\mathrm{h}}(\mathbb{C}^{2d})$*. Then* $\mathrm{e}^{-D} \in Sp_{\mathrm{h}}(\mathbb{C}^{2d})$*.*
(4) *Let* $D \in sp_{\mathrm{p}}(\mathbb{C}^{2d})$*. Then* $\mathrm{e}^{-D} \in Sp_{\mathrm{p}}(\mathbb{C}^{2d})$*.*

Proof. Claims (1) and (3) are obvious corollaries from the definitions.

(2) Integrating

$$\frac{\mathrm{d}}{\mathrm{d}t}(\mathrm{e}^{-tD})^*\theta\mathrm{e}^{-tD} = -(\mathrm{e}^{-tD})^*(D^*\theta + \theta D)\mathrm{e}^{-tD} < 0, \tag{16.6}$$

we obtain $(\mathrm{e}^{-D})^*\theta\mathrm{e}^{-D} < \theta$.

(4) We can write

$$\mathrm{e}^{-D} = \mathrm{e}^{-\theta(\theta D)}.$$

We diagonalize simultaneously the positive form θD and θ. In the diagonalizing basis, the matrices θ and θD commute, the former has eigenvalues ± 1, the latter has positive eigenvalues. Hence e^{-D} has positive eigenvalues. □

17. Hamiltonians

Let $H \in \mathrm{Sym}(\mathbb{C}^{2d})$. As usual, the quadratic form $\mathbb{R}^{2d} \ni y \mapsto y^{\#}Hy \in \mathbb{C}$ will be also denoted by H. Let us briefly recall the properties of quantum quadratic Hamiltonians $\mathrm{Op}(H)$ and their relationship to the metaplectic group. We will use [11] as the basic reference, although most of these facts are well known.

Set

$$D := 2H\omega^{-1}. \tag{17.1}$$

Clearly, $D \in sp(\mathbb{C}^{2d})$. We will say that D is the *symplectic generator associated with the Hamiltonian* H.

First assume that $H \in \mathrm{Sym}(\mathbb{R}^{2d})$. It is well known that then $\mathrm{Op}(H)$ is essentially self-adjoint on $\mathcal{S}(\mathbb{R}^d)$ (see, e.g., [11, Theorem 10.21]). Moreover, $\mathrm{e}^{\mathrm{i}t\mathrm{Op}(H)} \in Mp(\mathbb{R}^{2d})$ (see, e.g., [11, Theorem 10.36]). Under the epimorphism 10.2, $\mathrm{e}^{\mathrm{i}t\mathrm{Op}(H)}$ is mapped onto e^{tD}, where $D \in sp(\mathbb{R}^{2d})$ is defined by (17.1) (see, e.g., [11, Theorem 10.22]). Finally, if $\mathrm{e}^{tD} \in Sp^{\mathrm{reg}}(\mathbb{R})$ and $C_t := c(\mathrm{e}^{tD})\omega^{-1}$,

$$\mathrm{e}^{\mathrm{i}t\mathrm{Op}(H)} = \sqrt{\det(1 + C_t\omega)}\mathrm{Op}(\mathrm{e}^{-\mathrm{i}C_t}), \tag{17.2}$$

see, e.g., [11, Theorem 10.35].

Next consider $H \in \mathrm{Sym}_{++}(\mathbb{C}^{2d})$. It is easy to show that $\mathrm{Op}(H)$ extends from $\mathcal{S}(\mathbb{R}^d)$ to a maximal accretive operator (see, e.g., [11, Theorem 10.21]). Moreover, $\mathrm{e}^{-t\mathrm{Op}(H)} \in \mathrm{Osc}_{++}^{\mathrm{nor}}(\mathbb{C}^{2d})$. In fact, if D is defined as in (17.1), then $-\mathrm{i}D \in sp_{++}(\mathbb{C}^{2d})$, and hence by Proposition 33(2), $\mathrm{e}^{\mathrm{i}tD} \in Sp_{++}(\mathbb{C}^{2d})$. Moreover, under the epimorphism (6.7), $\mathrm{e}^{-t\mathrm{Op}(H)}$ is mapped onto $\mathrm{e}^{\mathrm{i}tD}$. Finally, if we set $A_t := c(\mathrm{e}^{\mathrm{i}tD})\theta$, then

$$\mathrm{e}^{-t\mathrm{Op}(H)} = \sqrt{\det(\mathbb{1} + A_t\theta)}\mathrm{Op}(\mathrm{e}^{-A_t}), \tag{17.3}$$

see, e.g., in [11, Theorem 10.35].

18. Holomorphic 1-parameter subsemigroups

Let $H \in \mathrm{Sym}_{++}(\mathbb{C}^{2d})$. As we recalled above, $\mathrm{Op}(H)$ is maximally accretive, and hence

$$[0, \infty[\ \ni t \mapsto \mathrm{e}^{-t\mathrm{Op}(H)} \tag{18.1}$$

is a well defined subsemigroup of $\mathrm{Osc}_{++}(\mathbb{C}^{2d})$. One can ask whether it can be extended to a larger subsemigroup if we replace real t with a complex parameter.

If H is real, then the answer is obvious and simple. Then $\mathrm{Op}(H)$ is a positive self-adjoint operator and we have a well defined semigroup

$$\{z \in \mathbb{C} \mid \mathrm{Re}\, z \geq 0\} \ni z \mapsto \mathrm{e}^{-z\mathrm{Op}(H)} \tag{18.2}$$

inside $\mathrm{Osc}_{+}\big(\mathbb{C}^{2d}\big)$. For $\mathrm{Re}\, z > 0$, (18.2) is in $\mathrm{Osc}_{++}\big(\mathbb{C}^{2d}\big)$.

If H is not real, then the answer can be more complicated.

Let $D \in sp_{++}(\mathbb{C}^{2d})$ correspond to H as in (17.1). Clearly

$$\mathbb{C} \ni z \mapsto \mathrm{e}^{\mathrm{i}zD} \in Sp\big(\mathbb{C}^{2d}\big) \tag{18.3}$$

is a holomorphic subgroup of $Sp(\mathbb{C}^{2d})$. However, not all elements of the complex symplectic group correspond to (bounded) operators on the Hilbert space. Motivated by this, we define

$$\mathcal{A}_{+}(H) := \{z \in \mathbb{C} \mid \mathrm{e}^{\mathrm{i}zD} \in Sp_{+}\big(\mathbb{C}^{2d}\big)\}, \tag{18.4}$$

$$\mathcal{A}_{++}(H) := \{z \in \mathbb{C} \mid \mathrm{e}^{\mathrm{i}zD} \in Sp_{++}\big(\mathbb{C}^{2d}\big)\}. \tag{18.5}$$

From the definition it is obvious that $\mathcal{A}_{+}(H)$ is a closed subsemigroup of $\mathbb{C}$ and $\mathcal{A}_{++}(H)$ is an open subsemigroup of $\mathcal{A}_{+}(H)$.

If $z \in \mathcal{A}_{++}(H)$, then we define

$$A_z := c(\mathrm{e}^{\mathrm{i}zD})\theta \in \mathrm{Sym}_{++}\big(\mathbb{C}^{2d}\big), \tag{18.6}$$

$$\mathrm{e}^{-z\mathrm{Op}(H)} := \sqrt{\det(\mathbb{1} + A_z\theta)}\,\mathrm{Op}\big(\mathrm{e}^{-A_z}\big). \tag{18.7}$$

(The definition of (18.7) is consistent with the usual definition of $\mathrm{e}^{-z\mathrm{Op}(H)}$ for real positive z).

The shapes of $\mathcal{A}_{+}(H)$ and $\mathcal{A}_{++}(H)$ can be quite curious. This is already seen in the simplest nontrivial example, known under the name of the *Davies harmonic oscillator*, as shown in [1], see also [21]. In this example, $\psi \in\,]-\frac{\pi}{2}, \frac{\pi}{2}[$ is a parameter, the classical and quantum Hamiltonians and the generator are

$$H_\psi := \mathrm{e}^{\mathrm{i}\psi} x^2 + \mathrm{e}^{-\mathrm{i}\psi} p^2, \tag{18.8}$$

$$\hat{H}_\psi := \mathrm{Op}(H_\psi) = \mathrm{e}^{\mathrm{i}\psi}\hat{x}^2 + \mathrm{e}^{-\mathrm{i}\psi}\hat{p}^2, \tag{18.9}$$

$$D_\psi := 2\begin{bmatrix} 0 & -\mathrm{e}^{\mathrm{i}\psi} \\ \mathrm{e}^{-\mathrm{i}\psi} & 0 \end{bmatrix}. \tag{18.10}$$

The proposition below reproduces the result of Aleman and Viola (see (1.2) of [1]).

Proposition 34. *Let H_ψ be the Davies' harmonic oscillator, as above. Then*

$$\mathcal{A}_+(H_\psi) = \Big\{ z \in \mathbb{C} \mid \mathrm{Re}\,(z) \geq 0 \text{ and } |\arg\tanh z| + |\psi| \leqslant \frac{\pi}{2} \Big\}, \tag{18.11}$$

$$\mathcal{A}_{++}(H_\psi) = \Big\{ z \in \mathbb{C} \mid \mathrm{Re}\,(z) > 0 \text{ and } |\arg\tanh z| + |\psi| < \frac{\pi}{2} \Big\}. \tag{18.12}$$

Proof. $\mathrm{i}D_\psi$ generates a holomorphic group in $Sp\big(\mathbb{C}^{2d}\big)$, which can be computed using $D_\psi^2 = -4\mathbb{1}$ as

$$\mathrm{e}^{\mathrm{i}zD_\psi} = \begin{bmatrix} \cosh 2z & \mathrm{i}\mathrm{e}^{\mathrm{i}\psi} \sinh 2z \\ -\mathrm{i}\mathrm{e}^{-\mathrm{i}\psi} \sinh 2z & \cosh 2z \end{bmatrix}. \tag{18.13}$$

Now

$$A_{\psi,z} = c(\mathrm{e}^{\mathrm{i}zD_\psi})\theta = 2\tanh z \begin{bmatrix} \mathrm{e}^{-\mathrm{i}\psi} & 0 \\ 0 & \mathrm{e}^{\mathrm{i}\psi} \end{bmatrix}. \tag{18.14}$$

Let us denote $t := \arg\tanh z$. $A_{\psi,z}$ belongs to $\mathrm{Sym}_{++}\big(\mathbb{C}^{2d}\big)$ iff $\mathrm{Re}\,(z) > 0$ and

$$\begin{cases} |t+\psi| < \frac{\pi}{2}, \\ |t-\psi| < \frac{\pi}{2}. \end{cases} \tag{18.15}$$

The above pair of inequalities is equivalent to

$$|t| + |\psi| < \frac{\pi}{2}. \tag{18.16}$$

By Theorem 18(2), $A_{\psi,z} \in \mathrm{Sym}_{++}\big(\mathbb{C}^{2d}\big)$ iff $\mathrm{e}^{\mathrm{i}zD_\psi} \in Sp_{++}\big(\mathbb{C}^{2d}\big)$.

The proof for $\mathcal{A}_+\big(H_\psi\big)$ is analogous. □

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A resonance interaction of seismogravitational modes on tectonic plates

Victor Flambaum, Gaven Martin and Boris Pavlov

In memory of our colleague and friend Boris Sergeevich Pavlov

Abstract. This paper discusses resonance effects to advance a classical earthquake model, namely the celebrated M8 global test algorithm. This algorithm gives high confidence levels for prediction of Time Intervals of Increased Probability (TIP) of an earthquake. It is based on observation that almost 80% of earthquakes occur due to the stress accumulated from previous earthquakes at the location and stored in form of displacements against gravity and static elastic deformations of the plates. Nevertheless the M8 global test algorithm fails to predict some powerful earthquakes. In this paper we suggest the additional possibility of considering the dynamical storage of the elastic energy on the tectonic plates due to resonance beats of seismogravitational oscillations (SGO) modes of the plates. We make sure that the tangential compression in the middle plane of an "active zone" of a tectonic plate may tune its SGO modes to the resonance condition of coincidence the frequencies of the corresponding localized modes with the delocalized SGO modes of the complement. We also consider the beats arising between the modes under a small perturbations of the plates, and, assuming that the discord between the perturbed and unperturbed resonance modes is strongly dominated by the discord between the non-resonance modes estimate the energy transfer coefficient.

1. Exterior and interior dynamics of tectonic plates

The "M8 Global test algorithm" (see [12] and references) for earthquake prediction was designed in 1984 at the International Institute of Earthquake Prediction and Mathematical Geophysics (Moscow) based on the observation that almost 80% of actual events at the selected location arise due to the stress built up thanks to previous events at the corresponding earthquake-prone (active) zone. J.K. Gardner and L. Knopoff observed that a sequence of earthquakes in Southern California, with aftershocks removed, was Poissonian [7]. Since then a mix of statistical and

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analytical techniques through the results of a global 20-year long experiment gave indirect confirmation of common features of both the predictability and the diverse behaviour of the Earth's naturally fractal lithosphere. The statistics achieved to date prove (remarkably with confidence above 99%) the rather high efficiency of the M8 and M8-MSc predictions limited to intermediate-term middle- and narrow-range accuracy. These models also adaptable, see e.g. [25]. There are other models, we note those found in the works Turcotte and Schubert [35] and Dahlen and Tromp [5], and our ideas may have implications for these as well, though we do not give specific details here.

The analytical and mechanical arguments used to derive the various models are based on the assumption, that for the most part, the energy at the active zone is stored in the form of static elastic deformation and the displacement of tectonic plates in the gravitational field.

Though both M8 and the improved MSc algorithms are extremely efficient for prediction of the Time intervals of Increased Probability (TIP) of earthquakes, some highly dangerous events, such as the recent Tohoku earthquake (Japan,March 11, 2011) were not predicted. In Tohoku the "black box" constructed based on the above algorithms, removed the TIP warning from the list of expected earthquakes at the Tohoku location 70 days before the earthquake, see the retrospective analysis of the Global Test effectiveness given by Kossobokov in [14].

The mechanical arguments for these algorithms are derived from the idea of quasi-statical (adiabatic) variation of the potential energy of the plates during the periods between earthquakes while the tectonic plates participate in the "exterior" dynamics, such as floating of (fragments of) the plates down the slopes formed by previous earthquakes, or responding to the hydrodynamical oscillations in the resonance cavities at the earthquake-prone (active) zones filled with magma, see for instance, [31].

On the other hand, earthquakes do arise within a background formed by oscillations of the planet. Many seismologists study these typical oscillations with amplitudes within $\sim$ 0.2–0.5 cm, and periods of circa a few minutes. However interesting anomalies with periods of circa 10 minutes were noticed by G.A.Sobolev and A.A. Lyubushkin, see [32], in the course of their analysis of seismological data preceding the Sumatra earthquake on December 26, 2004, recorded *in the remote zone* of the earthquake. Moreover, some decaying periodic patterns, see Fig. 4 in [32], were noticed on the relevant spectral-temporal (time-spectral) cards, see below, with the periods $\sim$ 100 min. On diagram 7 of the same paper one can see decaying patterns with even greater periods $\sim$ 2400 min arising prior the major earthquake. Unfortunately the authors of [32] did not consider these as important details and did not develop any extended analysis of them in their paper.

Approximately a decade before this, see [18], long periodic oscillation patterns, with periods $\sim$ 40–70 minutes, were registered by E. M. Linkov using a "vertical pendulum", constructed especially for studying Seismogravitational Oscillations (SGO) of the Earth. These oscillations have been intensely monitored during the last decade, see, for instance, [27, 28], as an important component of the “interior dynamic” of the plates. They form a natural dynamical background of catastrophic events such as earthquakes, tsunami and volcanic eruptions. Monitoring of SGO confirmed the hypothesis [26, 29] of their spectral nature. According to [29], the SGO should be interpreted as decaying flexural (vertical) eigenmodes of large tectonic plates with linear size up to few thousands kilometers.

The typical energy of the mode may be estimated based on spectral (frequency), physical properties such as density and Young’s modulus and geometric characteristics of the plate. For instance, the elastic energy stored in a single SGO mode with frequency 200 μHz and amplitude 2×10^{-3} m on a tectonic plate with area circa 10^{14} m^2, thickness 10^5 m, and density 3380 kg m^{-3} is estimated as 54×10^9 J. This is almost equivalent to the seismic moment (“full energy”) of the 4M earthquake in Johannesburg (South Africa) of November 18, 2013.

While discussing the inner dynamics of tectonic plates in our recent publications, see [21, 6] and similarly [10], we proposed to take into account the migration of elastic energy between regions of tectonic plates, caused by beating of the resonance spectral modes localized on the regions. For an active zone, already unstable under statical stress, the migration of energy defined by the resonance beating might be sufficient to trigger an earthquake.

We therefore suggest that the modelling of tectonic processes with regard of resonance migration of energy would probably help in developing more realistic theoretical scenarios for an earthquake. In the simplest case of two resonance SGO modes, localized on neighbouring regions Ω_ε, Ω_c, the beating pattern is periodic and the amount of elastic energy transferred from one location to another on each period is defined by the corresponding *transfer coefficient.* The transfer coefficient may be large for exact tuning of the corresponding frequencies $|\nu_\varepsilon - \nu_c| \ll \bar{\nu} \equiv |\nu_\varepsilon + \nu_c|/2$. Thus we study the influence of resonance effects for this geophysical phenomenon and how t can be used to inform advances in the classical model and give examples which demonstrate that resonances can be a reason for earthquake. However we are not able to present a full model for the phenomenon. Some discussions pertain to one-dimensional systems and cannot present a completely realistic model, but they demonstrate the possibility of such mechanism in seismic phenomena as quite natural values of parameters are used. We hope the interested reader can follow the construction of the model and come to understanding of how full implementation might be realised. The examples we offer can be considered as benchmarks for future, more realistic models, based on these suggested ideas.

In this paper we aim at estimating the transfer coefficient, while considering the problem in frames of perturbation analysis, depending on the spectral characteristics of the unperturbed modes on disjoint regions and the type of interaction imposed. Usually the SGO modes are presented on time-spectral cards obtained from the corresponding seismograms via averaging of the SGO amplitudes, with certain frequency, on a step-wise system of time - windows, obtained by shifting an initial window by certain interval of time on each step. The boundaries of the spectral–time domains on the cards, where the averaged amplitude of the SGO mode exceeds the given value A, form a system of isolines in the frequency/time coordinates ν, T. The horizontal axis for time, is graded in hours, the vertical axis, for the frequencies, is graded in μHz. Doctor L. Petrova provided us with some time-spectral cards from her private collection and shared with us some useful and interesting comments concerning the interpretation of the cards in terms of SGO dynamics, which we referred in our previous publication [6]. Find below one of her cards which was obtained by her from seismograms recorded on SSB station, France, during the period preceding the powerful earthquake on 26 September, 2004 in Peru. The averaging of the amplitudes of the seismogravitational oscillations, with certain frequency, was done, after appropriate filtration, on a system of 20 hour time-windows, obtained by shifting an initial window by 30 minutes in each step. The relief of the window-averaged squared amplitude on the cards is graded by the isolines, with the step $\delta A^2 = \frac{1}{10}\left[A^2_{\max} - A^2_{\min}\right]$, and is painted accordingly between the isolines with shades depending on the square amplitude A^2 : dull grey for the background value $A^2_{\min}$ and white for the maximal value $A^2_{\max}$. See more comments in [6].

The most interesting kind of SGO was represented by *pulsations*, which were observed by Linkov's team as intense short (4–6 hours) and sometimes repeated in 30–100 hours, pulses of SGO with large amplitudes. Pulsations have been registered before 95% of powerful earthquakes and may be considered as natural precursors of them, see [18]. One may hope that a deeper analysis of the microseismic data in [32] would reveal a connection between the above "anomalies" with SGO and pulsation patterns studied by Linkov et al. Petrova pointed out to us a peculiar detail on the above SSB card above, consisting of two groups of stationary modes with almost equal frequencies and visually similar relief in $\Delta_2^{SSB} = (190, 200) \times (55, 65)$ and in $\Delta_3^{SSB} = (200, 210) \times (145, 165)$. The pair was interpreted by her as a typical "seismogravitational pulsation".

In [6] pulsations are interpreted as beatings of spectral modes on the tectonic plates, arising due to resonance interaction of the SGO modes, with close frequencies, while some of them are localized on active zone Ω_ε and others on the complement Ω_c. According to classical mechanics [15], the resonance between two "oscillators" $\Omega_{\varepsilon,\Omega_c}$ with close frequencies ω_ε, ω_c and precise tuning, the beating of a pair of modes defines the periodic energy migration between the regions $\Omega_{\varepsilon,\Omega_c}$: $E_\varepsilon(t) = \bar{E}_\varepsilon + \delta E(t)$, $E_c(t) = \bar{E}_c + \delta E(t)$. Here the migrating part $\delta E(t)$ of the total energy arises, with opposite phases, in both locations, with total energy conserved $E = \bar{E}_\varepsilon + \bar{E}_c$.

While two weakly connected oscillators in resonance yield a periodic beating, a larger group of oscillators, under resonance conditions $|\omega_i - \omega_k| \equiv \delta_{ik} \ll \overline{\Omega}$ with respect to the average frequency $\bar{\omega} \equiv \frac{1}{N}\sum_{k=1}^{N} \omega_k$ reveal a quasi-chaotic beating phenomenon, if the difference frequencies δ_{ik} are non-co-measurable.

The problem of estimation of the energy transfer associated with beats in the system of several connected oscillators can be reduced to the similar problem for a single oscillator under almost periodic resonance force. This is treated in Landau's

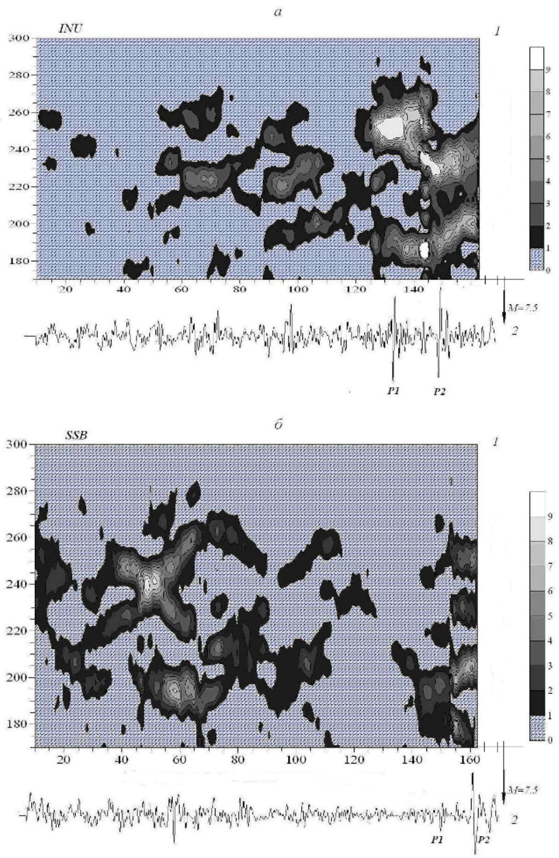

FIGURE 1. A time-spectral card

book [15, Sect. 22]. Indeed, we will consider two 1D oscillators, with masses m, M attached to springs v, V and connected by an hermitian pair of elastic bonds γ, Γ constrained by the Hermitian requirement $\gamma\ m^{-1} = \Gamma\ M^{-1} = \varepsilon$. For instance, a pair of oscillators the dynamics is described by the equations:

$$
\begin{aligned}
x'' + \frac{v}{m}x + \gamma\ m^{-1}X &= 0,\\
X'' + \frac{V}{M}X + \Gamma\ M^{-1}x &= 0.
\end{aligned}
\tag{1.1}
$$

While the elastic bonds are neglected, the eigenfrequencies of the oscillators can be calculated to be $\omega_m = \sqrt{v\, m^{-1}} \equiv \sqrt{\lambda_m},\ \omega_M = \sqrt{V\, M^{-1}} \equiv \sqrt{\lambda_M}$, but with regard of the bonds, they are found from the quadratic equation for $\lambda = \omega^2$, namely

$$\lambda_\pm = \frac{\lambda_m + \lambda_M}{2} \pm \sqrt{[\frac{\lambda_m + \lambda_M}{2}]^2 - \lambda_m \lambda_M + \varepsilon^2} = \frac{\lambda_m + \lambda_M}{2} \pm \sqrt{[\frac{\lambda_m - \lambda_M}{2}]^2 + \varepsilon^2}. \tag{1.2}$$

Hereafter we will assume that *the bonds are relatively weak* so that we may calculate the frequencies $\omega_\pm \equiv \sqrt{\lambda_\pm}$ of the normal modes of the pair approximately based on $\varepsilon \ll [\frac{\lambda_m - \lambda_M}{2}] \equiv \delta > 0$, at least up to second order with respect to $\varepsilon^2 [2\delta]^{-1}$:

$$\lambda_\pm = \frac{\lambda_m + \lambda_M}{2} \pm \frac{\lambda_m - \lambda_M}{2} \pm \frac{\varepsilon^2}{2\delta}. \tag{1.3}$$

This implies, up to second order with respect to $\varepsilon^2 [2\delta]^{-1}$:

$$\lambda_+ \approx \omega_m^2 + \varepsilon^2 \, [2\delta]^{-1}, \ \lambda_- = \omega_M^2 - \varepsilon^2 [2\delta]^{-1}$$

and allows us to calculate the complex normal modes with $\omega_\pm = \sqrt{\lambda_\pm}$ as

$$\begin{pmatrix} e_+ \\ E_+ \end{pmatrix} e^{\pm i\omega_+ t}, \ \begin{pmatrix} e_- \\ E_- \end{pmatrix} e^{\pm i\omega_- t}. \tag{1.4}$$

The eigenvectors $\begin{pmatrix} e_+ \\ E_+ \end{pmatrix}$ and $\begin{pmatrix} e_- \\ E_- \end{pmatrix}$ are found from the homogeneous equations

$$\begin{pmatrix} -\frac{\varepsilon^2}{2\delta} & \varepsilon \\ \varepsilon & -\delta - \frac{\varepsilon^2}{2\delta} \end{pmatrix} \begin{pmatrix} e_+ \\ E_+ \end{pmatrix} = 0, \ \begin{pmatrix} \delta + \frac{\varepsilon^2}{2\delta} & \varepsilon \\ \varepsilon & \frac{\varepsilon^2}{2\delta} \end{pmatrix} \begin{pmatrix} e_- \\ E_- \end{pmatrix} = 0, \tag{1.5}$$

which yield for the normalized eigenvectors, up to $O(\varepsilon^2 \ /\delta^2)$:

$$\begin{pmatrix} e_+ \\ E_+ \end{pmatrix} = \begin{pmatrix} 1 \\ \frac{\varepsilon}{2\delta} \end{pmatrix}, \ \begin{pmatrix} e_- \\ E_- \end{pmatrix} = \begin{pmatrix} -\frac{\varepsilon}{2\delta} \\ 1 \end{pmatrix}. \tag{1.6}$$

In [15] the beats phenomenon is considered for a harmonic external force. Hereafter we consider above system of two oscillators x, X, governed by the equations (1.1), under initial condition $x(0) = 1, x'(0) = 0, X(0) = \frac{\varepsilon}{2\delta}, X'(0) = 0$. These initial conditions correspond to an excitation of the normal mode of above the pair oscillators, with second order terms $\varepsilon^2\delta^{-2}$ neglected:

$$\begin{pmatrix} x_+(t) \\ X_+(t) \end{pmatrix} = \begin{pmatrix} 1 \\ \frac{\varepsilon}{2\delta} \end{pmatrix} \cos\omega_+ t. \tag{1.7}$$

Then the dynamics if the first oscillators may be considered under an exterior force:

$$x'' + \omega_m^2 x + \frac{\varepsilon^2}{2\delta} \cos\omega_+ \, t = 0, \ \text{with} \ \omega_+ = \omega_m + \frac{\varepsilon^2}{2\delta}, \tag{1.8}$$

under the initial conditions $x(0) = 1, x'(0) = 0$. Following [15], for the real solution of the above equation (1.7) we introduce a complex characteristic

$$\xi = x' + i\omega_m x, \tag{1.9}$$

and rewrite the above equation (1.8) for ξ as

$$\frac{d\xi}{dt} - i\omega_m + \frac{\varepsilon^2}{2\delta}\cos\omega_+ t, \tag{1.10}$$

and obtain the solution $\xi(t)$ as in [15]:

$$\xi(t) = e^{i\omega_m t}\left[\int_0^t \frac{\varepsilon^2}{2\delta}\cos\omega_+ \tau \ e^{i\omega_m \tau} d\tau + i\omega_m\right]. \tag{1.11}$$

The energy $\mathcal{E}(x)$ of the oscillator x is can be calculated as per [15] again, in terms of this characteristic as

$$\frac{m}{2}|\xi(t)|^2 = \frac{m}{2}\left[|x'|^2 + \omega_m^2|x|^2\right] = \mathcal{E}(x). \tag{1.12}$$

For two connected oscillators $\delta E(t)$, the migrating part of the total energy, is close to zero if the difference in frequency is relatively large. Vice versa, it may be close to the full energy if the tuning is very sharp, that is difference frequency is relatively small, $|\omega_i - \omega_k| \equiv \delta_{ik} \ll \overline{\omega}$. An example of this is the celebrated Wilberforce pendulum [36, 37, 2]. We posit that, in the case of tectonic plates, beating of the resonance SGO modes implies (depending on conditions) migration of an essential part $\max\delta E(t) = k\,E$ of the total energy E, with the transfer coefficient $k = k(\delta\omega/\omega)$, depending on the relative variation of the frequencies. Then the total energy of the active zone Ω_ε at some moment T_0 in time may exceed the destruction limit $E_\varepsilon(T) = \bar{E}_\varepsilon + \delta E(T_0) > E_\varepsilon^d$, causing the destruction of some structure in the active zone and thus triggering an earthquake.

Exactly this scenario was considered in [6] as a resonance mechanism for an earthquake. Comparison of the full energy of a single SGO mode with the seismic moment requires an estimation of the transfer coefficient k. This becomes an important question in analytic modelling of the resonance mechanism for an earthquake.

To obtain this estimation of the transfer coefficient k, in the next Sect. 2 we sketch the basics of the Kirchhoff model of the thin plate, which is used hereafter as the tectonic plate. We leave the matter of the hydrodynamical component of the dynamics and the dissipation to future work, and concentrate our attention here on the effect of the compressing (tangential) tension in the middle plane of the plate Ω_ε, causing a lowering of the eigenfrequencies of the active zone to the resonances with the SGO modes of the complement. Then in Section 3 we consider the resonance condition for the circular active zone, with the prescribed frequency 200 μHz, choosing typical physical and geometrical parameters of a pair Ω_ε, Ω_c of the disjoint plates. We consider the simplest explicitly solvable example of two unperturbed circular disjoint plates, and make sure that the resonance condition is fulfilled for the active zone Ω_ε, under the compressing tension, with the parameters properly chosen, and a circular plate Ω_c', while the tangential compression on the large plate is neglected in the resonance interval of frequencies. The circular large plate Ω_c' in Sect. 3 will differ from the actual complement Ω_c of the circular active zone Ω_ε in minor ways, dominated by the typical wavelengths of lower SGO modes on the plate. Hence so are the resonance conditions $\omega_c' \approx 200\ \mu$Hz $\approx \omega_c$. A more accurate analysis of the ring-like complement will be postponed to an appendix, where the Neumann-to-Dirichlet map of the ring is calculated in terms of Bessel functions. Similar arguments will work for the sectorial boundary active zone.

2. Modelling the resonance interaction between SGO and beating phenomena

This article investigates theoretical aspects of the resonance interaction of SGO modes based on the Kirchhoff model for a thin tectonic plate Ω, see [30], and the dynamics of the plate described by a perturbed biharmonic wave equation for vertical displacement $u(x,t)$:

$$H\rho u_{tt} + D\Delta^2 u + \nabla Q \nabla u = 0. \tag{2.1}$$

We formulate the appropriate boundary conditions on $\partial\Omega \equiv \Gamma$ which are derived from the corresponding Hamiltonian.

In (2.1) the flexural rigidity is

$$D = \frac{H^3 E}{12(1-\sigma^2)} \equiv D_H = D_1 \times H^3 = 1.56 \times H^3 \times 10^{10}\ \frac{\text{kg m}^2}{\text{s}^2}$$

is defined via

- Young modulus $E = 17.28 \times 10^{10}\ \frac{\text{kg}}{\text{m s}^2}$,
- Poisson coefficient $\sigma = 0.28$,
- thickness $H\ \sim 3 \times 10^4$–10^5 m, and
- density $\rho = 3380\ \frac{\text{kg}}{\text{m}^3}$ of the plate.

The tangential tension in the middle plane of the plate is modelled by the symmetric elliptic operator

$$\nabla Q \nabla u \equiv HTu \equiv \nabla Q_H \nabla u = H\left[T_x u_{xx} + 2T_{xy} u_{xy} + T_y u_{yy}\right] \equiv H \nabla Q_1 \nabla u,$$

as in [23, Chap. 4], and constrained in our case by the maximal non-destructing estimate from above $Q_1 \leq 0.3 \times 10^{10}$, see [6].

The boundary conditions for the biharmonic wave equation (2.1) are derived based on the Hamiltonian

$$\begin{aligned}\mathcal{E}(u) \quad = \quad & \frac{1}{2}\int_\omega \left[H\rho u_t^2 + D|\Delta u|^2 + 2D(1-\sigma)[|u_{xy}|^2 - u_{xx}u_{yy}] + \langle \nabla u, Q\nabla u\rangle\right] d\Omega \\ & + \frac{1}{2}\int_\Gamma \beta \left|\frac{\partial u}{\partial n}\right|^2 d\Gamma,\end{aligned}$$

see our Appendix 1, and a more detailed discussion in [23, Chaps. 4, 8], as well as [3], with regard to the boundary bending defined by an elastic bond $\beta\ \frac{\text{kg m}}{\text{s}^2}$.

The expression (2.2) can be transformed, under the Dirichlet boundary condition $u\big|_\Gamma = 0$ into the following equation:

$$\mathcal{E}_D(u) = \frac{1}{2}\int_\omega \left[H\rho u_t^2 + D|\Delta u|^2 + \langle \nabla u, Q\nabla u\rangle\right] d\Omega + \frac{1}{2}\int_\Gamma \left[\beta - D\frac{1-\sigma}{r}\right]\left|\frac{\partial u}{\partial n}\right|^2 d\Gamma, \tag{2.2}$$

where r is the curvature radius of the boundary (positive or negative depending on the position of the center of the curvature); see, for instance, [3].

Minimizing of the spacial part of the Hamiltonian (2.2) leads to the corresponding "natural" boundary conditions:

$$\left[\beta - D\frac{1-\sigma}{r}\right]\frac{\partial u}{\partial n} + D\Delta u\big|_\Gamma = 0. \tag{2.3}$$

Mikhlin proved, see [23], that the thin Kirchhoff plate is stable if $[\beta - D\frac{1-\sigma}{r}] \geq 0$ and $Q \geq 0$, corresponding to stretching in the middle plane. He also considered the contracting tension of the middle plane and found sufficient conditions for stability, see [23, Chaps. 5, 8]. Later Heisin [9] actually noticed in an experiment that that plates of ice are unstable with respect to certain contracting tension in the middle plane. In Sect. 3 we shall consider an example of a circular plates with centrally symmetric boundary conditions. The corresponding wave equations in the active zone Ω_ε are

$$H_\varepsilon \rho w_{tt} + D_\varepsilon \Delta^2 w + Q_\varepsilon \Delta w = 0, \tag{2.4}$$

and on the complement Ω_c. Here the tangent contraction in the middle plane is neglected ($Q_c = 0$), so that

$$H_c \rho w_{tt} + D_c \Delta^2 w + Q_c \Delta w = 0. \tag{2.5}$$

With properly selected parameters $H_\varepsilon = 3 \times 10^4$ m, $H_c = 10^5$ m, $D_\varepsilon = D_1 \times H_\varepsilon^3$, $D_c = D_1 \times H_c^3$..., solutions admit a spectral representation constructed with the use of Bessel functions.

In next section we ensure that the resonance condition $\lambda_\varepsilon = \lambda_c$ is satisfied for a pair of circular tectonic plates. In Sect. 4 we impose a weak bond onto a family of oscillators with a multiple eigenvalue and observe the dynamics of the corresponding perturbed system. It is this that exposes the beat phenomena involving the energy transfer between oscillators originally constrained by the resonance condition.

Ultimately we will estimate the transition coefficient for the energy transfer for the simplest solvable model of disjoint oscillators with relatively small masses and close frequencies $[\omega]$, perturbed by imposing a bond of them with an oscillator with larger mass M and frequency $\Omega \approx \omega$.

This leaves the challenging problem of realising this program for the calculation the energy transfer coefficient for oscillator's to the more interesting system of tectonic plates, based on fitted zero-range model. We may discuss this elsewhere.

3. Example: A circular active zone

Consider a thin circular plate Ω divided by a crack Γ_ε into two complementary parts: the circular active zone Ω_ε and the ring-like complement Ω_c, centred at Ω_ε.

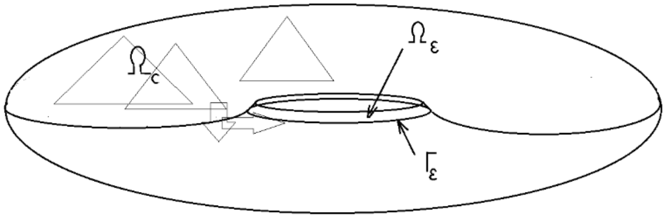

FIGURE 2. The small circular tectonic plate Ω_ε (the active zone) contacts the complementary large circular tectonic plate Ω_c along the boundary Γ_ε, while the large plate is loaded and covers the small plate on the contact line Γ_ε. Because of the load and the special geometry of the contact, the large plate develops a normal stress (vertical arrow) resulting in bending of the plate and a corresponding storage of elastic energy.

We begin with the case of disconnected parts, imposing on both sides of Γ_ε the kinematic boundary condition $w_\varepsilon\big|_\Gamma = w_c\big|_\Gamma = 0$ and independent free-reclining boundary conditions (see Appendix 1), or Neumann boundary conditions imposed on elements of the domain of the generators L_ε, L_c for the relevant biharmonic wave equations:

$$H\rho w_{tt} + D_\varepsilon \Delta^2 w + Q_\varepsilon \Delta w = H\rho w_{tt} + L_\varepsilon w = 0, \tag{3.1}$$

with tangential compression $Q_\varepsilon \Delta \equiv T$, $Q_\varepsilon > 0$, characterized by the positive scalar Q_ε and an elastic bond β applied on the boundary, as in (2.3):

$$w\big|_{\Gamma_\varepsilon} = 0, \quad \beta_\varepsilon \frac{\partial w}{\partial n} + D_\varepsilon \Delta w\big|_{\Gamma_\varepsilon} - \frac{D_\varepsilon(1-\sigma)}{\varepsilon}\frac{\partial w}{\partial n}\Big|_{\Gamma_\varepsilon} = 0. \tag{3.2}$$

On the complement Ω_c we neglect the tangential compression, $Q_c = 0$, but do keep the bending and the elastic bond

$$\rho H w_{tt} + D_c \Delta^2 w = \rho H w_{tt} + L_c w = 0, \tag{3.3}$$

for the boundary condition on the outer side of the crack Γ_ε

$$w\big|_{\Gamma_\varepsilon} = 0, \quad \beta_c \frac{\partial w}{\partial n} + D_c \Delta w\big|_{\Gamma_\varepsilon} - \frac{D_c(1-\sigma)}{\varepsilon}\frac{\partial w}{\partial n}\Big|_{\Gamma_\varepsilon} = 0, \tag{3.4}$$

and for the boundary condition on the remote part Γ_a of the boundary of ring-like complement Ω_c we have

$$\Psi_c\Big|_{\Gamma_a} = 0, \quad \left[D_c \frac{1-\sigma}{r} - \beta_c\right] \frac{\partial \Psi_c}{\partial n} - D_c \Delta \Psi_c\Big|_{\Gamma_a} = 0. \tag{3.5}$$

The spectral characteristics of the generators L_ε and L_c of the wave dynamics on both $\Omega_\varepsilon, \Omega_c$, for given geometrical and physical parameters can be recovered by separation of variables.

We attempt to select the parameters $D_\varepsilon = H^3_{\varepsilon \times D_1}, \varepsilon, Q_\varepsilon = H_\varepsilon \times Q_1$ with regard of the resonance frequency $\nu_0 = 2 \times 10^{-4}$ Hz and later choose the outer radius a of the complement Ω_c such that one of ground frequencies of the biharmonic generator L_c also coincides with $\nu_0 = 2 \times 10^{-4}$ Hz. Then the so constructed pair of operators L_ε, L_c can be perturbed by the connecting boundary condition on the crack, such that the multiple eigenvalue $\omega_0^2 = 4\pi^2 \nu_0^2$ would split into a starlet $\omega_0^2 \longrightarrow \omega_0^2 \left(1 + \delta[\alpha]\right), [\alpha] = [\alpha_1, \alpha_2]$ as described below, implementing the beating of corresponding spectral modes on Q_ε, Q_c.

All data, except the radius ε of the active zone and the outer radius of the complement, are selected as in the previous section, but we may assume the freedom of an adiabatic change, with time, of the tangent tension in the middle plane as $Q_1 = qH \times 10^9,\ 1 \leq q < 3$ below the destruction limit of the active zone Ω_ε, implying the change of eigenfrequencies $\omega_\varepsilon(q)$ of the active zone depending on the compressing tension.

Removing the common factor H_ε from the coefficients of the wave equation on the active zone Q_ε and from the boundary conditions we obtain an equivalent form of (3.1) and the spectral problem on Ω_ε with $H = H_\varepsilon$:

$$D_1 H^2 \Delta^2 w + Q_1 \Delta w = \omega^2 \rho w, \quad \frac{\partial w}{\partial n}\Big|_{\Gamma_\varepsilon} = u\Big|_{\Gamma_\varepsilon} = 0. \tag{3.6}$$

In our earlier work [6] we estimated the small eigenvalues of the above equations neglecting the boundary effects. This is acceptable for large plates, see [6], but we notice that improved results can be obtained based on a more accurate spectral analysis of the biharmonic generator L_ε, using a factorization of the above equation with Dirichlet–Neumann boundary conditions at the crack:

$$\begin{aligned} 0 = &\left[-\sqrt{D_1} H \Delta - \frac{Q_1}{2\sqrt{D_1} H} - \sqrt{\Omega^2 \rho + \frac{Q_1^2}{4 D_1 H^2}}\right] \\ &\times \left[-\sqrt{D_1} H \Delta - \frac{Q_1}{2\sqrt{D_1} H} + \sqrt{\Omega^2 \rho + \frac{Q_1^2}{4 D_1 H^2}}\right] \end{aligned} \tag{3.7}$$

For the circular active zone Ω_ε and centrally symmetric $w = \Psi_\varepsilon,\ \Delta \equiv \Delta_0$ is the corresponding radial Laplacian, hence the above equation (3.7) has a solution vanishing on $\Gamma_\varepsilon : r = \varepsilon$ presented as a linear combinations of Bessel functions and modified Bessel functions with appropriate arguments:

$$\Psi_\varepsilon(r) = \frac{J_0\left(\left[\frac{\omega^2\rho}{H^2 D_1}e^{2\Theta}\right]^{1/4} r\right)}{J_0\left(\left[\frac{\omega^2\rho}{H^2 D_1}e^{2\Theta}\right]^{1/4} \varepsilon\right)} - \frac{I_0\left(\left[\frac{\omega^2\rho}{H^2 D_1}e^{-2\Theta}\right]^{1/4} r\right)}{I_0\left(\left[\frac{\omega^2\rho}{H^2 D_1}e^{-2\Theta}\right]^{1/4} \varepsilon\right)}. \tag{3.8}$$

Here $\sinh\Theta = \frac{Q_1}{2\omega H\sqrt{D_1\rho}}$ reveals the dependence of the resonance on the tangential tension Q. Besides

$$-\Delta J_0\left(\left[\frac{\omega^2\rho}{D}e^{2\Theta}\right]^{1/4} r\right) = \left[\frac{\omega^2\rho}{D_1 H^2}e^{2\Theta}\right]^{1/2} J_0\left(\left[\frac{\omega^2\rho}{D}e^{2\Theta}\right]^{1/4} r\right),$$

$$\Delta I_0\left(\left[\frac{\omega^2\rho}{D}e^{-2\Theta}\right]^{1/4} r\right) = \left[\frac{\omega^2\rho}{D_1 H}e^{-2\Theta}\right]^{1/2} I_0\left(\left[\frac{\omega^2\rho}{D_1 H^2}e^{-2\Theta}\right]^{1/4} r\right).$$

We are interested in small positive eigenvalues ω^2 of the equation (3.6) which may be in resonance with the lower eigenmodes of the complementary part Ω_c of the plate. To recover an algebraic equation for the eigenfrequencies we substitute the spectral parameter ω by a new spectral parameter Θ connected to ω by the equation

$$\sinh\Theta = \frac{Q}{2\omega\sqrt{D\rho}},$$

or

$$\omega \equiv \frac{Q}{2\sinh\Theta\sqrt{D\rho}} = \frac{Q}{\left[e^{\Theta} - e^{-\Theta}\right]\sqrt{D\rho}}, \quad \Theta > 0.$$

The unperturbed spectral problem with the new spectral parameter is defined by the Dirichlet–Neumann boundary condition while constructed of Bessel functions as

$$\Psi_\varepsilon(r) = \frac{J_0\left(e^{\Theta/2}\frac{\sqrt{Q}}{\sqrt{D}\sqrt{e^{\Theta}-e^{-\Theta}}}r\right)}{J_0\left(e^{\Theta/2}\frac{\sqrt{Q}}{\sqrt{D}\sqrt{e^{\Theta}-e^{-\Theta}}}\varepsilon\right)} - \frac{I_0\left(e^{-\Theta/2}\frac{\sqrt{Q}}{\sqrt{D}\sqrt{e^{\Theta}-e^{-\Theta}}}r\right)}{I_0\left(e^{-\Theta/2}\frac{\sqrt{Q}}{\sqrt{D}\sqrt{e^{\Theta}-e^{-\Theta}}}\varepsilon\right)}, \tag{3.9}$$

and satisfies zero boundary condition identically on the inner side of the crack Γ_ε. The Neumann boundary condition on the inner side of the crack is

$$\begin{aligned}\frac{\partial\Psi_\varepsilon}{\partial n}(\varepsilon) = e^{\Theta/2}\frac{\sqrt{Q_1}}{\sqrt{D_1 H^2}\sqrt{e^{\Theta}-e^{-\Theta}}}\frac{J_0'\left(e^{\Theta/2}\frac{\sqrt{Q_1}}{\sqrt{D_1 H^2}\sqrt{e^{\Theta}-e^{-\Theta}}}\varepsilon\right)}{J_0\left(e^{\Theta/2}\frac{\sqrt{Q_1}}{\sqrt{D_1 H^2}\sqrt{e^{\Theta}-e^{-\Theta}}}\varepsilon\right)} \\ - e^{-\Theta/2}\frac{\sqrt{Q_1}}{\sqrt{D_1 H^2}\sqrt{e^{\Theta}-e^{-\Theta}}}\frac{I_0\left(e^{-\Theta/2}\frac{\sqrt{Q_1}}{\sqrt{D_1 H^2}\sqrt{e^{\Theta}-e^{-\Theta}}}\varepsilon\right)}{I_0\left(e^{-\Theta/2}\frac{\sqrt{Q_1}}{\sqrt{D_1 H^2}\sqrt{e^{\Theta}-e^{-\Theta}}}\varepsilon\right)} = 0\end{aligned} \tag{3.10}$$

and defines the spectrum of the unperturbed Dirichlet–Neumann problem for selected values of the parameters involved.

We select the typical geometrical and physical parameters of the active zone Ω_ε as

- $D_1 \times H^2 = 1.56 \times 10^{10} \times H^2 \ \frac{\text{kg m}}{\text{s}^2}$,
- $H = H_\varepsilon \sim 3 \times 10^4$ m,
- $\rho = 3380 \ \frac{\text{kg}}{\text{m}^3}$, $\sigma = 0.28$, $Q \approx 3 \times 10^9 \frac{\text{kg}}{\text{m s}}$, and
- $\varepsilon = \text{radius} \cdot \Omega_\varepsilon \sim 2.6 \times 10^5$ m

(with a little bit of accurate tuning). Then we are able to substitute the Bessel functions J_0 and the corresponding derivatives by the asymptotics for "large" values of the argument, and I_0 and the corresponding derivatives by the asymptotics for small ones, with regard of the factor $e^{-\Theta}$, calculated for the selected resonance frequency $\nu = 2 \times 10^{-4}$ Hz of the lower eigenmodes of large tectonic plates.

$$\sinh \Theta = \frac{Q}{4\pi\nu\sqrt{\rho D}} = \frac{3 \times 10^9}{12.56 \times 2 \times 10^{-4} \times 3 \times 10^4 \times 1.26 \times 10^5} = 5.5,$$

and $e^\Theta = 11$. Then the arguments of the Bessel functions and their derivatives can be calculated to be

$$J_0\left(\omega^{1/2}\left(\frac{\rho}{D}\right)^{1/4} e^{\Theta/2}\varepsilon\right) = J_0\left(\left[\frac{12.6 \times 10^{-4} \times 58 \times 11 \times 6.76 \times 10^{10}}{1.26 \times 10^5 \times 3 \times 10^4}\right]^{1/2}\right)$$
$$\approx J_0\left(\frac{\sqrt{1505}}{10}\right) = J_0(3.9), \tag{3.11}$$

$$I_0'\left(\omega^{1/2}\left(\frac{\rho}{D}\right)^{1/4} e^{\Theta/2}\varepsilon\right) = I_0\left(\left[\frac{12.6 \times 10^{-4} \times 58 \times 6.76 \times 10^{10}}{1.26 \times 10^5 \times 11 \times 3 \times 10^4}\right]^{1/2}\right)$$
$$\approx I_0\left(\frac{\sqrt{61}}{10}\right) \approx I_0(0.8). \tag{3.12}$$

Hereafter we use standard Taylor asymptotics of the modified Bessel function I_0 for small values of argument (< 1) and the exponential asymptotics for "large" arguments (≥ 3.9) in J_0,

$$J_0(z) \approx \frac{\cos(z - \pi/4) + O(1/z)}{\sqrt{\frac{\pi z}{2}}}, \qquad J_0'(z) \approx \frac{-\sin(z - \pi/4) + O(1/z)}{\sqrt{\frac{\pi z}{2}}},$$
$$I_0(z) \approx \frac{\cosh z + O(1/z)}{\sqrt{\frac{\pi z}{2}}}, \qquad I_0'(z) \approx \frac{\sinh z + O(1/z)}{\sqrt{\frac{\pi z}{2}},}. \tag{3.13}$$

Then we notice that the equation (3.10) is satisfied, with data, selected above, up to an error ~ 0.1. This means that our guess concerning the magnitude of the frequency was reasonably accurate for an active zone with radius 2.6×10^5 with standard physical characteristics and circular shape.

A more profound correspondence between the interval 150–250 μHz of typical frequencies and various shapes of the active zone requires a further analysis of the corresponding dispersion equation (analogue of 3.10) and is postponed.

4. Resonance conditions for circular plates

To reveal the resonance condition for the circular plate divided into two parts: the circular active zone Ω_ε and the ring-like complement $\Omega_c = \{\varepsilon < r < a\}$, which is centered at Ω_ε and elastically disconnected from the active zone due to independent Dirichlet–Neumann conditions on both sides of the common boundary Γ_ε we must select the geometrical parameters of the complement such that the disconnected spectral problem has a multiple eigenvalue $\omega_0^2 = 4\pi^2\nu_0 62$. Then the perturbation of the disconnected spectral problem defined by replacing the disconnecting boundary conditions by an interactive condition would reveal a splitting of the multiple eigenvalue, and, eventually, the the resonance beating of SGO modes, localized on $\Omega_\varepsilon, \Omega_c$. This would imply migration of energy between the locations. It is technically convenient to consider a circular pate Ω_c' with the same outer radius a, but without a hole reserved for Ω_ε at the center. The perturbation obtained by replacement $\Omega_c \to \Omega_c'$ should not affect the part of spectrum corresponding to the standing waves in which lengths exceed the geometric size of the details affected by the change, in our case the radius 2.6×10^5 m of the hole Ω_ε (the active zone). This condition is obviously satisfied for ground SGO modes on the disc Ω_c' with $R \approx 5000$ m. Now estimation of the eigenfrequencies of the complement for an equivalent circular plate Ω_c', with radius $a \approx 5 \times 10^6$ m, neglecting relatively small terms, compared with the typical ground flexural wavelengths $2a \approx 5 \times 10^6$ m, the hole radius ε. We assume for $\Omega_c, \Omega_c' : D_a = 1.56 \times 10^{10} \times H_a^2 \, \frac{\text{kg m}}{\text{s}^2}$, $H_a = H_c \sim 10^5$ m, $Q_c \approx 0$ and $\rho = 3380 \, \frac{\text{kg}}{\text{m}^3}$. We also use of the asymptotics of the derivatives of the Bessel functions for the solutions Ψ_a of the spectral problem

$$D_a \Delta^2 w = \omega^2 \rho w \tag{4.1}$$

on the complement, with $Q_c = 0$, $\Theta_c = 0$:

$$\Psi_a(r) = \frac{J_0\left(\left[\frac{\omega^2\rho}{D_1 H_a^2}\right]^{1/4} r\right)}{J_0\left(\left[\frac{\omega^2\rho}{D_1 H_a^2}\right]^{1/4} a\right)} - \frac{I_0\left(\left[\frac{\omega^2\rho}{D_1 H_a^2}\right]^{1/4} r\right)}{I_0\left(\left[\frac{\omega^2\rho}{D_1 H_a^2}\right]^{1/4} a\right)}. \tag{4.2}$$

For the Neumann dispersion equation on the remote part Γ_a of the boundary,

$$\frac{\partial \Psi_a}{\partial n}(\varepsilon) \times \sqrt{\frac{\pi z}{2}} = \frac{J_0'\left(\sqrt{\omega}\left(\frac{\rho}{D_1 H_a^2}\right) a\right)}{J_0\left(\sqrt{\omega}\left(\frac{\rho}{D_1 H_a^2}\right) a\right)} - \frac{I_0'\left(\sqrt{\omega}\left(\frac{\rho}{D_1 H_a^2}\right) a\right)}{I_0\left(\sqrt{\omega}\left(\frac{\rho}{D_1 H_a^2}\right) a\right)} = 0. \tag{4.3}$$

Using the asymptotics of Bessel functions for large arguments on the remote part of the boundary $r = a$ we find that

$$\frac{I_0'\left(\sqrt{\omega}\left(\frac{\rho}{D_1 H_a^2}\right) a\right)}{I_0\left(\sqrt{\omega}\left(\frac{\rho}{D_1 H_a^2}\right) a\right)} \approx 1 = -\tan \pi \left(l - \frac{1}{4}\right),$$

$$\frac{J_0'\left(\sqrt{\omega}\left(\frac{\rho}{D_1 H_a^2}\right)^{1/4} a\right)}{J_0\left(\sqrt{\omega}\left(\frac{\rho}{D_1 H_a^2}\right)^{1/4} a\right)} \approx -\tan\left(0.6a \times 10^{-7} - \frac{\pi}{4}\right).$$

This results in $0.6a \times 10^{-7} - \pi/4 = \pi l - \pi/4$ and hence $a \approx 5 \times 10^6$ m, for $l = 1$ in agreement with our preliminary guess.

More detailed estimation of the radius of the ring-like complement $\Omega_c \equiv (\varepsilon < r < a)$, centered at the active zone Ω_ε may be derived from an explicit construction of the basic Bessel solutions and the Neumann-to-Dirichlet map of the biharmonic d'Alambert equation (4.1) on the ring with and appropriate symmetry, compatible with typical standing waves on the complement.

$$J_p(z) \approx \frac{\cos(z - p\pi/2 - \pi/4)}{\sqrt{\pi z/2}} + O\big(|1/z|\big)e^{|\Im z|},$$

$$J_p'(z) \approx \frac{-\sin(z - p\pi/2 - \pi/4)}{\sqrt{\pi z/2}} + O\big(|1/z|\big)e^{|\Im z|},$$

$$I_p(z) \approx \frac{e^z}{\sqrt{\pi z/2}} + O\big(e^{|\Im z|}\big), \tag{4.4}$$

$$I_p'(z) \approx \frac{e^z}{\sqrt{\pi z/2}} + O\big(e^{|\Im z|}\big). \tag{4.5}$$

One can also consider a circular active zone on an arbitrary plate with smooth boundary, see [33], or derive the formulae for the ND-map based on integral equation techniques, see [3].

Henceforth we wish to consider sectorial circular active zones which admit a separation of variable along with solutions of the relevant perturbed biharmonic equation

$$D\Delta^2 u + Q\Delta u = \omega^2 \rho u \tag{4.6}$$

combined on the sector $\Omega_\varepsilon^p : 0 \le r < \varepsilon,\ 0 < \varphi < \pi/p$ of above Bessel functions with index p and the corresponding circular harmonics $\cos p\phi$, $\sin p\phi$ on the sector, as above.

The roles of basic regular solutions of the biharmonic d'Alambert equation play the products of circular harmonics $\sin p\phi, \cos p\phi$, with relevant Bessel functions $\mathcal{J}_p\big(r\sqrt{\omega}\left(\frac{\rho}{D}\right)^{-1/4} e^{\Theta/2}\big)$, and the modified Bessel functions

$$\mathcal{I}_p\left(r\sqrt{\omega}\left(\frac{\rho}{D}\right)^{-1/4} e^{-\Theta/2}\right).$$

The parameter Θ is derived from the factorization of the d'Alambert equation as at (3.7). Then, for $p \geq 1$ the only continuous at $r = 0$ solution are square integrable. Hence continuous solutions of the d'Alambert equation, vanishing on the circular part Γ_ε of the boundary can b obtained as linear combinations.

$$\Psi_s(r) = \sin p\phi \left[\frac{J_p\left(\left[\frac{\omega^2\rho}{D}e^{2\Theta}\right]^{1/4} r\right)}{J_p\left(\left[\frac{\omega^2\rho}{D}e^{2\Theta}\right]^{1/4} \varepsilon\right)} - \frac{I_p\left(\left[\frac{\omega^2\rho}{D}e^{-2\Theta}\right]^{1/4} r\right)}{I_p\left(\left[\frac{\omega^2\rho}{D}e^{-2\Theta}\right]^{1/4} \varepsilon\right)} \right], \tag{4.7}$$

$$\Psi_c(r) = \cos p\phi \left[\frac{J_\gamma\left(\left[\frac{\omega^2\rho}{D}e^{2\Theta}\right]^{1/4} r\right)}{J_p\left(\left[\frac{\omega^2\rho}{D}e^{2\Theta}\right]^{1/4} \varepsilon\right)} - \frac{I_p\left(\left[\frac{\omega^2\rho}{D}e^{-2\Theta}\right]^{1/4} r\right)}{I_p\left(\left[\frac{\omega^2\rho}{D}e^{-2\Theta}\right]^{1/4} \varepsilon\right)} \right]. \tag{4.8}$$

They satisfy the Dirichlet boundary conditions $u\big|_\Gamma = \Delta u\big|_\Gamma = 0$ for Ψ_s and the Neumann boundary condition $\frac{\partial u}{\partial n}\Big|_\Gamma = \frac{\partial \Delta u}{\partial n}\Big|_\Gamma = 0$, respectively.

The spectral problem with Dirichlet–Neumann boundary condition $u\big|_{\Gamma_\varepsilon} = \frac{\partial u}{\partial n}\Big|_{\Gamma_\varepsilon}$ on the circular part of the boundary is given by linear combinations (4.7), (4.8), and which satisfy the corresponding dispersion equations:

$$\begin{aligned} 0 = \frac{\partial \Psi_s}{\partial n}(\varepsilon)\, \sin\gamma\phi & \left[e^{\Theta/2} \frac{\sqrt{Q}}{\sqrt{D}\sqrt{e^\Theta - e^{-\Theta}}} \frac{J'_\gamma\left(e^{\Theta/2}\frac{\sqrt{Q}}{\sqrt{D}\sqrt{e^\Theta - e^{-\Theta}}}\varepsilon\right)}{J_\gamma\left(e^{\Theta/2}\frac{\sqrt{Q}}{\sqrt{D}\sqrt{e^\Theta - e^{-\Theta}}}\varepsilon\right)} \right. \\ & \left. - e^{-\Theta/2} \frac{\sqrt{Q}}{\sqrt{D}\sqrt{e^\Theta - e^{-\Theta}}} \frac{I'_\gamma\left(e^{-\Theta/2}\frac{\sqrt{Q}}{\sqrt{D}\sqrt{e^\Theta - e^{-\Theta}}}\varepsilon\right)}{I_\gamma\left(e^{-\Theta/2}\frac{\sqrt{Q}}{\sqrt{D}\sqrt{e^\Theta - e^{-\Theta}}}\varepsilon\right)} \right], \end{aligned} \tag{4.9}$$

or a similar equation for Ψ_c.

For sectors characterized by $p \in (0, 1)$ there are singular square-integrable solutions $J_{-p}(z),\ I_{-p}(z)$ of the biharmonic d'Alambert equation, see [4]. Then we are able to consider the singular (discontinuous) square integrable solutions of the biharmonic d'Alambert equation, considering them as elements of the corresponding defect, see [4], and construct self-adjoint extensions of the corresponding biharmonic operator in the space of square-integrable functions in an sectorial active zone on the boundary. The corresponding operator extension machinery can be developed with use of extension procedure, similar to one developed above for the inner zero-range active zone.

When varying the tension parameter Q, we will come to the moment when the tangent compression in the middle plane is large enough for the minimal eigenvalue on the active zone of an unperturbed problem to coincide with an eigenvalue of the biharmonic spectral problem ($Q = 0$) on the complement. At this point substituting the asymptotics of the Bessel functions J_p, I_p for large and small values of the arguments, one can obtain an estimation for the contracting tension Q, this leads to the resonance conditions for the operators L_ε, L_c on $\Omega_\varepsilon, \Omega_c$, without an interaction between them. We now explore this in the simplest case.

5. A simple model of alternation

Now we consider a simple universal interaction depending on a small parameter between similar operators constructed for the zero-range active zone. Based on this construction, we observe the relevant beating phenomenon and estimate the transfer coefficient.

The system of two tectonic plates considered in the previous section is a special case of a decoupled oscillator's system under the resonance conditions. The interaction between the plates could be introduced by imposing free reclining or natural boundary conditions.

We now make some simplifying assumptions: we consider a weakly coupled oscillatory system obtained by attaching one (supposedly "large") multi-dimensional oscillator $X = (X_1, X_2, X_3, \ldots, X_\mu) \in C_\mu$ to a 1D (supposedly "small") oscillator characterized by the coordinate $x = x_1 \in C_1$.

The dynamics of the resulting system is defined by the system of linear equations

$$\begin{aligned} m x_{tt} + v x + b^+ X &= 0, \\ M X_{tt} + V X + b x &= 0. \end{aligned} \tag{5.1}$$

Here $m = m_1, v = v_1, M = [M_1, M_2, M_3 \ldots M_\mu], V = [V_1, V_2, V_3, \ldots, V_\mu]$, are positive diagonal matrices acting in the Hilbert spaces C_1, C_μ, $C_1 \xrightarrow{b} C_\mu$, $C_\mu \xrightarrow{b^+} C_1$. Interaction of the oscillators is introduced by the Hermitian matrix $B : C_1 \oplus C_\mu \longrightarrow C_1 \oplus C_\mu \equiv K$

$$B = \begin{pmatrix} 0 & b^+ \\ b & 0 \end{pmatrix} \equiv \text{antidiag}\left(b^+, b\right), \tag{5.2}$$

which plays the role of bonds imposed on the boundary data of solutions of the biharmonic equation on the border of the tectonic plate. Separating time, we obtain the spectral problem corresponding to the above wave equation (5.1), namely

$$\begin{aligned} v x + b^+ X &= m \lambda x \\ V X + b x &= M \lambda X. \end{aligned} \tag{5.3}$$

To make this consistent with the above model of tectonic plates supplied with natural structure of active zones we assume that the unperturbed multidimensional oscillator has a family of unperturbed eigenvalues (square frequencies) $[\omega^0]^2 =$

v/m, $\left[\Omega_s^0\right]^2 = V_s/M_s, s = 1, 2, \ldots, \mu$. For non-zero interaction $B \neq 0$ the eigenvalues $\lambda_r^b = (\omega_r^b)^2$ (and the corresponding eigenfrequencies) of the perturbed selfadjoint spectral problem are found from the algebraic equation

$$[\lambda m - v]\, a + b^+ \frac{I}{V - M\lambda} ba \equiv \mathcal{M}(\lambda) a = 0, \tag{5.4}$$

obtained via the elimination of X from the second equation in (5.3). In particular, for the 1D case, $\mu = 1$, we have two unperturbed frequencies

$$v/m = \omega^0 \equiv (\omega_1^0)^2, \quad V/M = \Omega^0 \equiv (\omega_2^0)^2$$

and a quadratic equation for the perturbed eigenvalues

$$\lambda_r^b = (\omega_r^b)^2, \quad r = 1, 2,$$

while the unperturbed are $\lambda_1^0 = (\omega^0)^2$, $\lambda_2^0 = (\Omega^0)^2$. Denoting

$$\bar{\lambda}^0 = \frac{(\omega^0)^2 + (\Omega^0)^2}{2}, \quad \delta\lambda^0 = \left| \frac{(\omega^0)^2 - (\Omega^0)^2}{2} \right|,$$

we find the perturbed frequencies/eigenvalues $\lambda_r^b \equiv (\omega_r^b)^2$ from the quadratic equation

$$\lambda^2 - 2\lambda\, \delta\lambda^0 + \lambda_1^0\, \lambda_2^0 = \frac{b^2}{mM}.$$

This gives

$$\lambda_r^b = \bar{\lambda}^0 \pm h, \text{ with } h^2 = (\delta\lambda)^2 + \frac{b^2}{mM},$$

with $m_1 = m$, $m_2 = M$. We further assume that $\frac{b^2}{m_1 m_2} \ll \delta^2\lambda$. This assumption allows us to calculate the perturbed eigenvalues $\lambda_{1,2}^b$ with $h = \delta\lambda + \frac{b^2}{2m_1\, m_2\, \delta\lambda}$ approximately. These turn out to be

$$\begin{aligned}
\lambda_{1,2}^b &= \lambda_{1,2}^0 \pm \frac{b^2}{2m_1\, m_2\, \delta\lambda}, \\
\omega_{1,2}^b &= \omega_{1,2}^0 \pm \frac{b^2}{4m_1\, m_2\, \delta\lambda\, \omega_{1,2}^0} = \omega_{1,2}^0 \left[1 \pm \frac{b^2}{4m_1\, m_2\, \delta\lambda^2}\right] \frac{\delta\lambda}{\lambda_{1,2}^0} \approx \omega_{1,2}^0 \frac{\delta\lambda}{\lambda_{1,2}^0}.
\end{aligned} \tag{5.5}$$

Generally, for $\mu \geq 1$, the eigenvalues of the ultimate spectral problem $\lambda = \lambda_1^b, \lambda_2^b, \ldots, \lambda_s^b, \ldots, \lambda_{1+\mu}^b$ may be found from the corresponding determinant condition. The components of the corresponding eigenvectors $\left\{a, \Psi_s^b\right\} \equiv \mathbf{\Psi}_s^b$ in K, C_μ are calculated from the equation

$$\Psi_s^b = \left(V - M\lambda_s^b\right)^{-1} ba, \tag{5.6}$$

with an appropriate normalization $m|a|^2 \left[1 + \langle M \frac{I}{V - M\lambda} b, \frac{I}{V - M\lambda} b\rangle\right] = 1$. If the interaction b is real and the initial data of the relevant Cauchy problem, see below (5.9), are real, then the corresponding solution is real, too. Similarly the solution of the corresponding inhomogeneous equation, with a real function in the right side, is real as well.

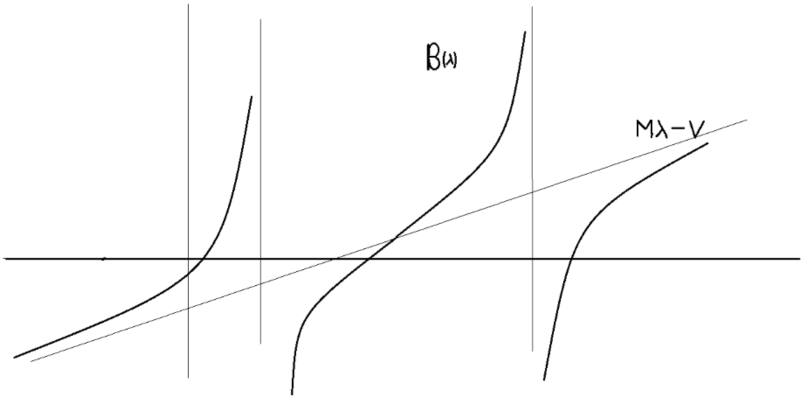

FIGURE 3. In the more general case where $K = C_1 \oplus C_\mu$, $\mu \geq 1$, the eigenvalues $\lambda_s^b = (\omega_s^b)^2$ are found as graphical solutions based on the diagram, corresponding to the algebraic equation (5.4), see [13].

In the simplest situation where $\mu = 1, K = C_1 \oplus C_1$, equation (5.3) for $(u, U) = (u_1, u_2)$ and the unperturbed frequencies $\omega^0 \equiv \omega_1^0, \Omega^0 = \omega_2^0$ and

$$\bar{\lambda} = \frac{\lambda_1^0 + \lambda_2^0}{2}, \quad \delta\lambda = \frac{\lambda_1^0 - \lambda_2^0}{2}$$

can be represented as

$$\begin{pmatrix} m_1\lambda_1^0 & b^+ \\ b & m_2\lambda_2^0 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \end{pmatrix} = \lambda \begin{pmatrix} m_1 & 0 \\ 0 & m_2 \end{pmatrix} \begin{pmatrix} u_1 \\ u_2 \end{pmatrix}, \tag{5.7}$$

and the eigenvectors

$$\mathbf{\Psi}_1^b = \begin{pmatrix} a_1 \\ \frac{a_1 b m_2^{-1}}{-\delta\lambda - h} \end{pmatrix}, \ \mathbf{\Psi}_2^b = \begin{pmatrix} a_2 \\ \frac{a_2 b m_2^{-1}}{-\delta\lambda + h} \end{pmatrix} \tag{5.8}$$

are orthogonal with respect to diag (m_1, m_2) and normalized in $l_2(m_1, m_2)$ with $a_{1,2} = \sqrt{\frac{h \pm \delta\lambda}{2h}}$. When discussing the general case $\mu \geq 1$ we may assume that the eigenfunctions $\mathbf{\Psi}_s^b = \left(\psi_s^b, \Psi_s^b\right)$ of the perturbed spectral problem (5.3) correspond to simple eigenvalues and are orthogonal and normalized. Using the eigenvectors, the normal modes of the wave equation

$$\begin{aligned} m u_{tt} + v u + b^+ U = 0, \\ M U_{tt} + V U + b u = 0, \\ (u, U) \equiv \mathbf{U}, \ \mathbf{U(0)} = \mathbf{U_0}, \ \frac{\mathbf{dU}}{\mathbf{dt}}(\mathbf{0}) = \mathbf{U}_0'. \end{aligned} \tag{5.9}$$

can be constructed, and subsequently the solutions of this Cauchy problem (5.9) are obtained as linear combinations

$$\mathbf{U}(t) = \sum_s U^s \boldsymbol{\Psi}_s \cos(\omega_s^b t + \varphi_s) = \Re \sum_s U^s \boldsymbol{\Psi}_s e^{i(\omega_s^b t + \varphi_s)}$$

of the eigenmodes. But we also can reduce the above homogeneous equation (5.9) to a pair of unperturbed formally inhomogeneous equations,

$$m u_{tt} + v u + \sum_s U^s \; b^+ \Psi_s \; \cos(\omega_s^b t + \varphi_s) \equiv m u_{tt} + v u + f, \tag{5.10}$$

$$M\, U_{tt} + V U + \sum_s U^s \; b \; \psi_s^b \; \cos(\omega_s^b t + \varphi_s) \equiv M\, U_{tt} + V U + F = 0, \tag{5.11}$$

or a similar complex equation

$$m \vec{u}_{tt} + v \vec{u} + \sum_s U^s \; b^+ \Psi_s \; e^{i(\omega_s^b t + \varphi_s)} \equiv m \vec{u}_{tt} + v \vec{u} + \vec{f}, \tag{5.12}$$

$$M\, \vec{U}_{tt} + V \vec{U} + \sum_s U^s \; b \; \psi_s^b \; e^{i(\omega_s^b t + \varphi_s)} \equiv M\, \vec{U}_{tt} + V \vec{U} + \vec{F} = 0, \tag{5.13}$$

with inhomogeneities $\vec{f} = b^+ U, \vec{F} = b\vec{u}$ obtained via substitution, for u, U, the corresponding components of the solution $\mathbf{U}(t) = (u, U)$ of the Cauchy problem (5.9) for the original oscillators system:

$$u_{\vec{f}}(t) = \sum_s b^+ \; \Psi_s \, U^s \left[\frac{e^{i(\omega_s^b t + \varphi_s)}}{m \lambda_s^b - v} \right], \; u_f(t) = \sum_s b^+ \; \Psi_s \, U^s \left[\frac{\cos(\omega_s^b t + \varphi_s)}{m \lambda_s^b - v} \right], \tag{5.14}$$

$$U_{\vec{F}}(t) = \sum_s b \, \psi_s \, U^s \left[\frac{e^{i(\omega_s^b t + \varphi_s)}}{M \lambda_s^b - V} \right], \; U_F(t) = \sum_s b \, \psi_s \, U^s \left[\frac{\cos(\omega_s^b t + \varphi_s)}{M \lambda_s^b - V} \right]. \tag{5.15}$$

General solutions of the equations (5.10)–(5.13) are obtained by adding general solutions of the corresponding homogeneous equations

$$m u_{tt} + v u = 0, \quad M\, U_{tt} + V U = 0,$$

to the solutions of the inhomogeneous equations.

The last formulas allow us to calculate partial values of energy of the "small" and "large" oscillators depending on time, for instance,

$$E_f(U) = \frac{m |u_f'|^2 + v |u_f|^2}{2}, \quad E_F(U) = \frac{M |U_F'|^2 + V |U_F|^2}{2} \tag{5.16}$$

under formally "exterior" forces f, F, defined by a linear combination of the perturbed normal modes $\mathbf{U}$ of the perturbed oscillator's system.

The partial values of energy of each oscillator u_f, U_F do not remain constant in the course of evolution, but depend on time, exposing beats while the oscillators exchange energy due to the bond $B = \text{antidiag}(b^+, b)$. Beats are calculated using the 1D theory developed for a periodic exterior force as in [15, Sect. 22]. To study the above (formally) complex version of the inhomogeneous equation (5.13) we follow Landau [15], and introduce the data $\vec{\xi}_f = \sqrt{m}\ u'_{\vec{f}} + i\sqrt{v}\ u_{\vec{f}},\ \xi_f = \sqrt{m}\ u'_f + i\sqrt{v}\ u_f$ and rewrite the last equation (5.12) as

$$\sqrt{m}\ \vec{\xi'} - i\sqrt{v}\ \vec{\xi} = \vec{f}(t), \quad \sqrt{m}\ \xi' - i\sqrt{v}\ \xi = f(t), \quad \sqrt{v} = \omega^0\sqrt{m}. \tag{5.17}$$

If the Cauchy problem is solved, with an initial condition $\xi(0) = \xi_0$, then the energy (5.16) of the small oscillator for the real solution $\mathbf{U}$ of the total problem, is calculated as

$$\bar{\xi}_f(t)\ \xi_f(t) = \overline{[\sqrt{m}u' + i\sqrt{v}u]}\ [\sqrt{m}u' + i\sqrt{v}u] = 2E_f(u). \tag{5.18}$$

The last formula allows us to estimate the energy transfer "between the modes of unperturbed oscillators". It is sufficient to be able to monitor the time-depndent energy of the small oscillator.

We now suggest a 1D version of the corresponding analysis, assuming that $\mu = 1,\ K = C_1 \oplus C_1$. Back to discussion of the 1D oscillators, with $\lambda^b_{1,2} = \bar{\lambda} \pm h \equiv \lambda^b_{\pm}$, assume, that an approximate resonance condition is satisfied,

$$\omega^b_{1,2} = \omega^0_{1,2} + \frac{b^2}{4m_1\, m_2\, \delta\lambda\omega^0_{1,2}},$$

and assume that the solution of the original Cauchy problem (5.9) is given as a linear combination of the perturbed modes

$$\mathbf{U} = \begin{pmatrix} u \\ U \end{pmatrix} = \sum_{s=1}^{2} \mathbf{\Psi}^b_s U^s \cos(\omega^b_s t + \varphi_s).$$

Then the above inhomogeneous evolution equation for the small oscillator is either

$$m_1 u_1^{''} + m(\omega^0)^2 u_1 + \sum_{s=1}^{2} b^+ \Psi^b_s U^s \cos(\omega^b_s t + \varphi_s) = 0,$$

or

$$\sqrt{m}\ [\xi' - i\omega^0_1 \xi] + \sum_{s=1}^{2} b^+ \Psi^b_s U^s \cos(\omega^b_s t + \varphi_s) = 0,$$

and has a partial solution

$$u_1 = \sum_{s=1}^{2} b^+ \Psi^b_s U^s \frac{\cos(\omega^b_s t + \varphi_s)}{m_1\, [(\omega^b_s)^2 - (\omega^0_1)^2]}.$$

The corresponding ξ-function is calculated from the equation

$$\sqrt{m}\ [\xi'_1 - i\xi_1\omega^0_1] + \sum_{s=1}^{2} b^+ \Psi^b_s U^s \cos(\omega^b_s t + \varphi_s) = 0,$$

as

$$\xi_1(t) = e^{i\omega_1^0 t}\left[\xi_1(0) - \frac{1}{\sqrt{m_1}}\int_0^t e^{-i\omega_1^0 \tau}\sum_{s=1}^{2} b^+\Psi_s^b U^s \cos(\omega_s^b\tau + \varphi_s)d\tau\right] \\ \equiv e^{i\omega_1^0 t}\left[\xi_1(0) + \hat{\xi}_1(t)\right], \tag{5.19}$$

with

$$\begin{aligned}\xi_1(0) &= \sqrt{m_1}\left[u'{}_1(0) + i\omega_1^0 u_1^0(0)\right] \\ &= \frac{1}{\sqrt{m_1}}\sum_{s=1}^{2} b^+\Psi_s^b U^s \frac{\left[-\omega_s^b \sin\varphi_s + i\omega_1^0 \cos\varphi_s\right]}{[(\omega_s^b)^2 - (\omega_1^0)^2]} \\ &= \frac{1}{\sqrt{m_1}}\sum_{s=1}^{2} b^+\Psi_s^b U^s \left[\frac{\sin\varphi_s}{\omega_1^b + \omega_1^0} + \frac{i\omega_1^0 e^{i\varphi_s}}{(\omega_s^b + \omega_1^0)(\omega_s^b - \omega_1^0)}\right]\end{aligned}$$

and the integral $\hat{\xi}_1(t)$ in (5.19) is calculated as

$$\begin{aligned}\hat{\xi}_1(t) &= -\frac{1}{\sqrt{m_1}}\int_0^t e^{-i\omega_1^0 \tau}\sum_{s=1}^{2} b^+\Psi_s^b U^s \cos(\omega_s^b\tau + \varphi_s)d\tau \\ &= -\frac{1}{\sqrt{m_1}}\sum_{s=1}^{2} b^+\Psi_s^b U^s \\ &\quad \cdot\left[\frac{e^{i\varphi_s}}{2i(\omega_s^b - \omega_1^0)}\left(e^{i(\omega_s^b - \omega_1^0)t} - 1\right) - \frac{e^{-i\varphi_s}}{2i(\omega_s^b + \omega_1^0)}\left(e^{i(-\omega_s^b - \omega_1^0)t} - 1\right)\right] \\ &= -\frac{1}{\sqrt{m_1}}\sum_{s=1}^{2} b^+\Psi_s^b U^s \\ &\quad \cdot\left[e^{i\varphi_s}\, e^{i(\omega_s^b - \omega_1^0)\frac{t}{2}}\, \frac{\sin(\omega_s^b - \omega_1^0)\frac{t}{2}}{\omega_s^b - \omega_1^0} + e^{-i\varphi_s}\, e^{-i(\omega_s^b + \omega_1^0)\frac{t}{2}}\, \frac{\sin(\omega_s^b + \omega_1^0)\frac{t}{2}}{\omega_s^b + \omega_1^0}\right].\end{aligned}$$

To compare the above theoretical estimation of time dependence of the energy of the "small" oscillator of time, we should consider the averaged energy over a stepwise system of windows, such as used for manufacturing the time-spectral cards discussed in Sect. 1. Set

$$\overline{|\xi|^2}(T) = \frac{1}{\Delta}\int_{T-\Delta/2}^{T+\Delta/2} |\xi(t)|^2 dt, \tag{5.20}$$

with an appropriate choice of parameters for the averaging depending on the basic characteristics of $\lambda_{1,2}$ or $\bar{\lambda}, \delta\lambda$.

Let us first examine the time-dependence of energy of the "small"oscillator in the simplest case of two 1D oscillators, we assume, that there exists only one resonance eigenvalue of the perturbed system, closest to the unperturbed eigenvalue of the "small" oscillator. Further assuming that $\frac{b^2}{m_1\, m_2} \ll (\delta\lambda)^2$, we may estimate the perturbed eigenvalues and eigenfrequencies of the system as

$$(\omega_1^b)^2 - (\omega_1^0)^2 \approx \bar{\lambda} + \sqrt{(\delta\lambda)^2 + \frac{b^2}{m_1\, m_2}} - \lambda_1^0 = \frac{b^2}{2m_1\, m_2\, \delta\lambda\, \lambda_1^0},$$

$$(\omega_2^b)^2 - (\omega_1^0)^2 \approx \bar{\lambda} - \sqrt{(\delta\lambda)^2 + \frac{b^2}{m_1\, m_2}} - \lambda_1^0 = -\delta\lambda - \frac{b^2}{2m_1\, m_2\, \delta\lambda\, \lambda_2^0}, \quad (5.21)$$

$$\omega_1^b - \omega_1^0 \approx \frac{b^2}{4m_1\, m_2\, \delta\lambda\, \omega_1^0}, \quad \omega_1^b + \omega_1^0 \approx 2\omega_1^0 + \frac{b^2}{4m_1\, m_2\, \delta\lambda\, \omega_1^0},$$

$$\omega_2^b - \omega_1^0 \approx \omega_2^0 - \omega_1^0 - \frac{b^2}{4m_1\, m_2\, \delta\lambda\, \omega_2^0} \equiv \delta\omega - -\frac{b^2}{4m_1\, m_2\, \delta\lambda\, \omega_2^0}. \quad (5.22)$$

Notice the resonance terms with small denominators or/and with slowly oscillating exponents on the window give the crucial contribution to the average (5.20) while the rapidly oscillating and smooth terms may be neglected while integrating over the window. Using the above representation for $\xi_1(t) = \xi_1(0) + \hat{\xi}(t)$ we estimate the averaged ξ-function $\overline{|\xi|^2}(T)$

$$\begin{aligned} \overline{|\xi|^2}(T) &= \frac{1}{\Delta} \int_{T-\Delta/2}^{T+\Delta/2} |\xi(t)|^2 dt \\ &= \frac{1}{m_1} \sum_{r,s=1}^{2} b^+ \Psi_r^b U^r \; b^+ \Psi_s^b U^s \frac{1}{\Delta} \int_{T-\Delta/2}^{T+\Delta/2} \overline{A} B, \end{aligned} \quad (5.23)$$

where

$$A = \frac{\sin\varphi_s}{\omega_s^b + \omega_1^0} + \frac{i\omega_1^0 e^{i\varphi_s}}{\lambda_s^b - \lambda_1^0} + \left[e^{i\varphi_s} e^{i(\omega_s^b - \omega_1^0)\frac{t}{2}} + e^{-i\varphi_s} e^{-i(\omega_s^b + \omega_1^0)\frac{t}{2}} \right] \frac{\sin(\omega_s^b + \omega_1^0)\frac{t}{2}}{\omega_s^b + \omega_1^0},$$

$$B = \frac{\sin\varphi_r}{\omega_r^b + \omega_1^0} + \frac{i\omega_1^0 e^{i\varphi_r}}{\lambda_r^b - \lambda_1^0} + \left[e^{i\varphi_r} e^{i(\omega_r^b - \omega_1^0)\frac{t}{2}} + e^{-i\varphi_r} e^{-i(\omega_r^b + \omega_1^0)\frac{t}{2}} \right] \frac{\sin(\omega_r^b + \omega_1^0)\frac{t}{2}}{\omega_r^b + \omega_1^0},$$

choosing the window such that the leading resonance term $\frac{\sin(\omega_r^b - \omega_1^0)\frac{t}{2}}{\omega_r^b - \omega_1^0}$ only slightly deviates from a constant on the window $|t - \tau| < \Delta$:

$$\left| \sin(\omega_r^b - \omega_1^0)\frac{t}{2} - \sin(\omega_r^b - \omega_1^0)\tau/2 \right| \leq \Delta(\omega_r^b - \omega_1^0) \approx \frac{b^2\ \Delta}{4m_1 m - 2\delta\lambda\omega_1^0}.$$

On another hand, the slowest oscillation of non-resonance exponentials in the integrand is defined by the exponent

$$\frac{1}{\Delta} \int_{T-\Delta/2}^{T-\Delta/2} cos(\omega_s^b - \omega_1^0) t dt \approx \frac{1}{\Delta\ \delta\omega}$$

and this should be small too:

$$\frac{b^2\ \Delta}{4m_1 m_2 \delta\lambda\omega_1^0} \approx \frac{1}{\Delta\ \delta\omega}.$$

This now defines the width of the optimal window giving the dependence on λ_1^0, λ_2^0 and the other parameters.

Then, selecting this optimal window and taking into account only leading terms of the integrand, we obtain an approximate estimation for the averaged energy of the "small" oscillator in dependence on time:

$$\begin{aligned} |\bar{\xi}|(T) &= \frac{1}{\Delta}\int_{T-\Delta/2}^{T+\Delta/2} |\xi|^2(t)dt \\ &\approx |b^+\Psi^s U^s|^2 dt \left[\frac{|\omega_1^0|^2}{\lambda_1^b - \lambda_1^0} + \frac{\sin^2(\omega_1^b - \omega_1^0)\frac{t}{2}}{(\omega_1^b - \omega_1^0)^2}\right] \\ &\approx |b^+\Psi^s U^s|^2 \left[\frac{2m_2\delta\lambda\lambda_1^0}{b^2} + \frac{\sin^2(\frac{b^2}{4m_1\, m_2\delta\lambda\omega_1^0})}{(\frac{b^2}{4m_1\, m_2\delta\lambda\omega_1^0})^2}\right]. \end{aligned} \tag{5.24}$$

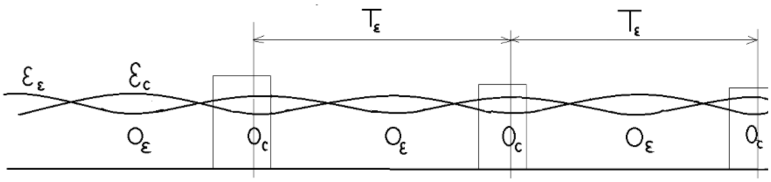

FIGURE 4. Symbolic diagram of the energy content $\mathcal{E}_\varepsilon(T)$, $\mathcal{E}_c(T)$ of the components $u_{\varepsilon,c}$ of the perturbed dynamics u with respect to the de-localized mode Ψ_c^0 on the complement Ω_c and one of the localized mode on the active zone Ω_ε. Positions O_ε, O_c of the minima (and maxima) of the energy content of the localized and the delocalized modes alternate with opposite phases. The dangerous intervals of time at the minima O_c, when the destruction of Ω_ε is expected, are marked with thin rectangles.

6. Appendix 1: Natural boundary conditions and the perturbed biharmonic wave equation

In our Sect. 2 we considered a perturbed biharmonic equation (2.1), borrowed from [9, 23], and modelled the normal stress by the boundary condition. Here we give more details describing the "bridge" connecting the model dynamics presented in by us with the corresponding chapter of classical mechanics of the plates and shells, see [33, 34, 23] and also [8, 11]. We keep in mind, that the linear theory of small oscillations of tectonic plates will only shed light on an initial phase of the process which may lead to the catastrophic results. But we hope that the the mechanical realization of the preliminary small oscillation model of the resonance process may be able to preview some initial features of the catastrophic phase of the process. In reality, constructing the mechanical model of the resonance interaction of the SGO modes of tectonic plates is a problem to resolve based on experiment, with use of far more detailed mechanical details, see for instance [34, 30, 22]. We only attempt here a first step in this direction, by considering two thin tectonic plates developing typical kinds of stresses when colliding under fluctuation of the rotation speed of Earth an/or the convection flow in the liquid underlay (astenosphere). To further simplify our analysis, we assume that both $\Omega_\varepsilon, \Omega_c$ are Kirchhoff plates, see [34], and endure different kinds of stresses. We assume that the normal pressure and the corresponding bending dominate the potential energy of the large plate Ω_ε and the tangential (shearing) component of the stress dominates the potential energy of the small plate. The shearing part of the stress is defined by the tension T in the middle plane of with the components T_x, T_y, T_{xy}, satisfying the equilibrium conditions, see Mikhlin's book [23, Chap. 4, Sect. 28] which we use as a basic reference in what comes. The equilibrium conditions are

$$\frac{\partial T_x}{\partial x} + \frac{\partial T_{xy}}{\partial y} = 0, \quad \frac{\partial T_y}{\partial y} + \frac{\partial T_{xy}}{\partial x} = 0, \tag{6.1}$$

and the corresponding quadratic form

$$\langle w, Tw \rangle = \int_{\Omega_\varepsilon} \left[w_x T_x w_x + 2 w_x T_{xy} w_y + w_y T_y w_y \right] d\Omega$$

defines, with the kinematic boundary condition $w\big|_\Gamma = 0$, a symmetric operator T of second order on smooth functions w. Operator T is positive for stretching tension and negative for compressing tension, see [9].

This may cause an instability of the tectonic plate, see for instance the analysis of a numerical example for an elliptic plate under a compressive tension in [23, Chap. 8, Sect. 72]. The materials composing tectonic plates can't resist the stretching tension, so hereafter we assume that the tension T is compressing, and the corresponding second order operator T is negative.

We begin with considering of the non-interacting plates $\Omega_\varepsilon, \Omega_c$ under normal bending stress F, and the compressing stress T, assuming that each of them is elastically fixed at the common boundary Γ_ε, see below. The zero boundary condition is applied on all boundaries, free reclining conditions are applied on the remote part of boundary of Ω_c, and the elastic fixture on both sides $\Gamma_{\varepsilon,c}$ of the common boundary Γ is modeled by the corresponding functionals $\int_\Gamma \beta_{\varepsilon,c} \left(\frac{\partial w_{\varepsilon,c}}{\partial n} \right)^2 d\Gamma$.

The equilibrium deformations w_ε, w_c are found by minimizing of the corresponding quadratic functionals on the subspace of the virtual strains, subject to the kinematic boundary condition $w\big|_{\Gamma_\varepsilon} = 0$,

$$W(u) = D\int_\Omega |\Delta w|^2 d\Omega - 2(1-\sigma)D\int_\Omega \left(w_{xx}w_{yy} - |u_{xy}|^2\right) d\Omega + \int_\Gamma \beta\left(\frac{\partial w}{\partial n}\right)^2 d\Gamma + H\langle w, Tw\rangle - 2\int_\Omega wF d\Omega. \tag{6.2}$$

Here σ is the Poisson coefficient $0 < \sigma < 1$, D is the flexural ridigity, $D = \frac{H^2 E}{12(1-\sigma^2)}$, E is the Young modulus, H is the thickness of the plate, and $\beta > 0$ is the parameter defining the elastic contact of the plate with environment. The second integral of the Monge–Ampere form (the curvature of the surface $z = w(x,y)$) can be presented as an integral on the boundary, see [3], with regard of the above kinematic boundary condition $w\big|_\Gamma = 0$:

$$2\int_\Omega \left(w_{xx}w_{yy} - |w_{xy}|^2\right) d\Omega = \int_\Gamma \frac{\left(\frac{\partial w}{\partial n}\right)^2}{r(\gamma)} d\Gamma$$

For the circular Γ_ε we assume $r(\gamma) = \varepsilon$ and $H\langle w, Tw\rangle = H^{-2}D\Delta w$. Calculation of the first variation of the energy functional yields the Euler equation

$$D\Delta^2 w + Tw = F \tag{6.3}$$

with the kinematic and the natural (under the above elastic β-bound) condition on the each side of the common boundary, e.g.,

$$D\Delta w + \beta\frac{\partial w}{\partial n} - D\frac{1-\sigma}{r}\frac{\partial w}{\partial n}\bigg|_{\Gamma_\varepsilon} = 0. \tag{6.4}$$

To derive an equation for the small oscillation we consider, for each plate, the Lagrangian associated with the thin plate Ω, subject to the above elastic bound and the kinematic boundary conditions $u\big|_\Gamma = 0$,

$$\mathcal{L} = \int_0^t \int_\Omega D|\Delta w|^2 d\Omega\, dt - \int_0^t \int_\Omega \left[2D(1-\sigma)\left(w_{xx}w_{yy} - w_{xy}^2\right) - \rho H w_t^2\right] d\Omega\, dt + 2\int_0^t \int_\Gamma \beta\left(\frac{\partial w}{\partial n}\right)^2 d\Gamma dt + \int_0^T \langle w, Tw\rangle dt, \tag{6.5}$$

we obtain the perturbed biharmonic wave equation as the Euler equation for the critical points of the Lagrangian:

$$\rho H w_{tt} + D\Delta^2 w + Tw = 0, \tag{6.6}$$

with the "β-natural" free reclining boundary conditions on both sides of the common boundary

$$w\big|_\Gamma = 0, \quad D\Delta w + \beta\frac{\partial w}{\partial n} - \frac{D(1-\sigma)}{r}\frac{\partial w}{\partial n}\bigg|_\Gamma = 0, \tag{6.7}$$

and free reclining boundary condition on the complementary part of the boundary of Ω_c.

While considering a circular plate $\Omega : 0 < r < a$, assume that the active zone Ω_ε is centered in Ω, so that the complement Ω_c is a ring $0 < r < a$, as described earlier. Generally we have the Lagrangian

$$\mathcal{L} = \int_0^t \int_\Omega D|\Delta w|^2 d\Omega\, dt + \int_0^t \int_{\Gamma_\varepsilon} \beta \left(\frac{\partial w}{\partial n}\right)^2 d\Gamma_\varepsilon dt - \int_0^t \int_\Omega \rho H \left(\frac{\partial w}{\partial t}\right)^2 d\Omega\, dt$$
$$- 2D(1-\sigma) \int_0^t \left(w_{xx} w_{yy} - w_{xy}^2\right) d\Omega dt + \int_0^t \langle w, Tw\rangle dt, \tag{6.8}$$

This gives the perturbed biharmonic wave equation as the Euler equation for the critical points of the Lagrangian on Ω_c:

$$\rho H w_{tt} + D\Delta^2 w + Tw = 0, \tag{6.9}$$

and

$$\rho H w_{tt} + D\Delta^2 w + Tw = 0, \tag{6.10}$$

on Ω_ε, with $T < 0$ and the boundary condition with regard of the elastic bond:

$$w\big|_{\Gamma_\varepsilon} = 0, \quad \beta \frac{\partial w}{\partial n} D\Delta w\big|_{\Gamma_\varepsilon} - \frac{D(1-\sigma)}{\varepsilon} \frac{\partial w}{\partial n}\Big|_{\Gamma_\varepsilon} = 0.$$

For the complement we neglect the tangential compression, but keep the bending and the elastic bond, so that the Lagrangian is reduced to

$$\mathcal{L}_c = \int_0^T \int_\Omega D|\Delta w|^2 d\Omega\, dt + \int_0^T \int_{\Gamma_\varepsilon} \beta \left(\frac{\partial w}{\partial n}\right)^2 d\Gamma_\varepsilon dt - \int_0^T \int_\Omega \rho H \left(\frac{\partial w}{\partial t}\right)^2 d\Omega\, dt, \tag{6.11}$$

we obtain the perturbed biharmonic wave equation as Euler equation for the critical points of the Lagrangian L_c:

$$\rho H w_{tt} + D\Delta^2 w = 0, \tag{6.12}$$

with the boundary condition

$$w\big|_{\Gamma_c} = 0, \quad \beta \frac{\partial w}{\partial n} - D \frac{1-\sigma}{r} \frac{\partial w}{\partial n} + D\Delta w\big|_{\Gamma_\varepsilon} = 0.$$

We make now one more simplifying assumption, assuming that the operator L_ε on the active zone is defined on circular harmonics of zero order $n = 0$ (independent of the angular variable), and the operator L_c on the complement is defined on the linear span of circular harmonics of the first order, $e_1^c = \pi^{-1}\cos\varphi,\ e_1^s = \pi^{-1}\sin\varphi$, so that the corresponding eigenfunctions are spanned by the circular harmonics.

The unperturbed spectral problems, associated with the 1D differential equations

$$L_c^{c,s} w = D_c \Delta^2 w + Tw = \omega^2 H_c \rho w$$

have 4 linearly independent solutions $J_1, H_1^1 \equiv H_1, I_1, K_1$ with factors $\sin\varphi, \cos\varphi$.

We denote them by $J_1^{c,s}, H_1^{c,s}, I_1^{c,s}, K_1^{c,s}$.

Selecting appropriate elastic bonds, we may set the parameters $\beta_0, \beta_1^c, \beta_1^s$ so that the unperturbed spectral problems for $L_\varepsilon \oplus L_c^c \oplus L_c^s$ has a multiple eigenfrequency $\nu = (2\pi)^{-1}\omega$ for $\delta = 0$. Then the perturbed spectral problems, associated with the unperturbed operator

$$\begin{bmatrix} D\Delta_0^2 + Q\Delta & 0 & 0 \\ 0 & D\Delta_1^2 & 0 \\ 0 & 0 & D\Delta_1^2 \end{bmatrix} \equiv L_\varepsilon^0 \oplus L_1^c \oplus L_1^s$$

and separate β-natural boundary conditions on the common part of the boundary. For the perturbed problem, defined by the same differential expression

$$\begin{bmatrix} \beta_0 - D_\varepsilon \frac{1-\sigma}{r_\varepsilon} & \kappa^c e_0\rangle\langle e_1^c & \kappa^s e_0\rangle\langle e_1^s \\ \kappa^c e_1^c\rangle\langle e_0 & \beta_1^c - D_c \frac{1-\sigma}{r_\varepsilon} & 0 \\ \kappa^s e_1^s\rangle\langle e_0 & 0 & \beta_1^s - D_c \frac{1-\sigma}{r_\varepsilon} \end{bmatrix} \begin{bmatrix} \frac{\partial \Psi_0}{\partial n_c} \\ \frac{\partial \Psi_1^c}{\partial n_c} \\ \frac{\partial \Psi_1^s}{\partial n} \end{bmatrix} = \Delta \begin{bmatrix} \Psi_0 \\ \Psi_1^c \\ \Psi_1^s \end{bmatrix}. \qquad (6.13)$$

Here $\kappa^{c,s}$ are small real parameters. The multiple eigenfrequency is split into the starlet of simple perturbed eigenfrequencies with eigenfunctions constructed as linear combinations Ψ_0 of J_0, I_0 on Ω_ε, see Sect. 4, and a linear combination $\Psi_c^{c,s}$ of the $J_1^{c,s}, H_1^{c,s}, I_1^{c,s}, K_1^{c,s}$ with coefficients found from the above analog (6.13) of the free reclining boundary conditions and the unperturbed boundary condition on the complementary part of the boundary.

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On Positivity Preserving, Translation Invariant Operators in $L^p(\mathbb{R}^n)^m$

Fritz Gesztesy and Michael M.H. Pang

Dedicated, with admiration, to the memory of Boris Pavlov (1936–2016)

Abstract. We characterize positivity preserving, translation invariant, linear operators in $L^p(\mathbb{R}^n)^m$, $p \in [1,\infty)$, $m, n \in \mathbb{N}$.

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1. Introduction

This note should be viewed as an addendum to our paper [13], which was devoted to (conditional) positive semidefiniteness of matrix-valued functions and positivity preserving operators on spaces of matrix-valued functions. In the present note we consider the case of vector-valued functions.

More precisely, the scalar (i.e., $m = 1$) version of Corollary 3.3 in the present paper is presented in [21, Theorem XIII.52]. There are two intuitive ways to extend this classical result in [21] to matrix-valued functions F. One way is to consider $F(-i\nabla)$ and $\exp_H(tF)(-i\nabla)$ as multiplier operators on the matrix-valued L^2-space. This is what we have done in Theorem 4.11 of our earlier paper [13]. The second way is to consider $F(-i\nabla)$ and $\exp_H(tF)(-i\nabla)$ as multiplier operators on the vector-valued L^2 (and L^p) space. This is what we now have done in Corollary 3.3 in the present paper.

The prime motivation for us to study matrix-valued extensions of [21, Theorem XIII.52], and to write [13] and now the present paper, was to find a matrix-valued analog of the the Levy–Khintchine formula (cf. Theorem 2.2 (iv)). While this issue remains work in progress, we refer to the extensive literature devoted

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to matrix-valued Schrödinger operators cited, for instance, in [8, 9, 12], which underscores the interest in this subject.

To make this note somewhat self-contained, we summarize in Sect. 2 the necessary background material on (conditionally) positive semidefinite functions $F\colon \mathbb{R}^n \to \mathbb{C}$ (hinting briefly at some matrix-valued generalizations), and on Fourier multipliers in $L^1(\mathbb{R}^n)$ and $L^2(\mathbb{R}^n)$. Our principal result on positivity preserving, translation invariant, linear operators in $L^p(\mathbb{R}^n)^m$, $p \in [1,\infty)$, $m,n \in \mathbb{N}$, Theorem 3.2, and several corollaries are then treated in Sect. 3.

2. Some Background Material

In this preparatory section we briefly recall the basic definitions of (conditionally) positive semidefinite functions $F\colon \mathbb{R}^n \to \mathbb{C}$, and state two classical results in this context; we also briefly hint at a matrix-valued extension of Bochner's theorem (for details we refer to [13] and the extensive literature cited therein). Finally, we recall some results on Fourier multipliers in $L^1(\mathbb{R}^n)$ and $L^2(\mathbb{R}^n)$ (see [14, Sect. 2.5] for a detailed exposition).

However, before getting started, we briefly summarize the basic notation employed in this paper: The Banach space of bounded linear operators on a complex Banach space X is denoted by $\mathcal{B}(X)$.

For Y a set, Y^m, $m \in \mathbb{N}$, represents the set of $m \times 1$ matrices with entries in Y; similarly, $Y^{m\times n}$, $m,n \in \mathbb{N}$, represents the set of $m \times n$ matrices with entries in Y.

Unless explicitly stated otherwise, $\mathbb{C}^m$ is always equipped with the Euclidean scalar product $(\,\cdot\,,\,\cdot\,)_{\mathbb{C}^m}$ and associated norm $\|\,\cdot\,\|_{\mathbb{C}^m}$.

The symbol $\mathcal{S}(\mathbb{R}^n)$ denotes the standard Schwartz space of all complex-valued rapidly decreasing functions on $\mathbb{R}^n$. In addition, we employ the spaces,

$$C_0^\infty(\mathbb{R}^n) = \{f \in C^\infty(\mathbb{R}^n) \,|\, \operatorname{supp}(f) \text{ compact}\}, \tag{2.1}$$

$$C_\infty(\mathbb{R}^n) = \Big\{f \in C(\mathbb{R}^n) \,|\, \lim_{|x|\to\infty} f(x) = 0\Big\}. \tag{2.2}$$

Unless explicitly stated otherwise, the spaces (2.1)–(2.2) are always equipped with the norm $\|f\|_\infty = \operatorname{ess.sup}_{x\in\mathbb{R}^n}|f(x)|$.

For brevity, we will omit displaying the Lebesgue measure $d^n x$ in $L^p(\mathbb{R}^n)$, $p \in [1,\infty)\cup\{\infty\}$, whenever the latter is understood. The norm for $f = (f_1,\dots,f_m)^\top \in L^p(\mathbb{R}^n)^m$, $p \in [1,\infty)$, $m \in \mathbb{N}$, is defined by

$$\|f\|_{L^p(\mathbb{R}^n)^m} = \sum_{j=1}^m \|f_j\|_{L^p(\mathbb{R}^n)}, \quad f = (f_1,\dots,f_m)^\top \in L^p(\mathbb{R}^n)^m. \tag{2.3}$$

The symbols $L^p(\mathbb{R}^n)^m_+$ $\big($resp., $C_0^\infty(\mathbb{R}^n)^m_+\big)$ represent elements of $L^p(\mathbb{R}^n)^m$ $\big($resp., $C_0^\infty(\mathbb{R}^n)^m\big)$ with all entries nonnegative (Lebesgue) a.e.

The Fourier and inverse Fourier transforms on $\mathcal{S}(\mathbb{R}^n)$ are denoted by the pair of formulas,

$$(\mathcal{F}f)(y) = f^\wedge(y) = (2\pi)^{-n/2} \int_{\mathbb{R}^n} e^{-i(y\cdot x)} f(x)\, d^n x, \tag{2.4}$$

$$(\mathcal{F}^{-1}g)(x) = g^\vee(x) = (2\pi)^{-n/2} \int_{\mathbb{R}^n} e^{i(x\cdot y)} g(y)\, d^n y, \tag{2.5}$$
$$f, g \in \mathcal{S}(\mathbb{R}^n),$$

and we use the same notation for the appropriate extensions, where $\mathcal{S}(\mathbb{R}^n)$ is replaced by $L^p(\mathbb{R}^n)$, $p \in [1,\infty)$.

The open ball in $\mathbb{R}^n$ with center $x_0 \in \mathbb{R}^n$ and radius $r_0 > 0$ is denoted by the symbol $B_n(x_0, r_0)$, the norm of vectors $x \in \mathbb{R}^n$ is denoted by $\|x\|_{\mathbb{R}^n}$, the scalar product of $x, y \in \mathbb{R}^n$, is abbreviated by $(x,y)_{\mathbb{R}^n}$.

With $\mathfrak{M}_n$ the σ-algebra of all Lebesgue measurable subsets of $\mathbb{R}^n$ and for $E \in \mathfrak{M}_n$, the n-dimensional Lebesgues measure of E is abbreviated by $|E|$.

With the basic notation used in this paper now out of the way, we start our brief summary of the necessary background material and some of the results presented in [13].

Definition 2.1. *Let $m \in \mathbb{N}$, and $A \in \mathbb{C}^{m\times m}$, and suppose that $F\colon \mathbb{R}^n \to \mathbb{C}$, $n \in \mathbb{N}$.*

(i) A is called positive semidefinite, also denoted by $A \geqslant 0$, if

$$(c, Ac)_{\mathbb{C}^m} = \sum_{j,k=1}^{m} \overline{c_j}\, A_{j,k} c_k \geqslant 0 \ \text{ for all } \ c = (c_1, \dots, c_m)^\top \in \mathbb{C}^m. \tag{2.6}$$

(ii) $A = (A_{j,k})_{1\leqslant j,k\leqslant m} = A^* \in \mathbb{C}^{m\times m}$ is said to be conditionally positive semidefinite if

$$(c, Ac)_{\mathbb{C}^m} \geqslant 0 \ \text{ for all } \ c = (c_1, \dots, c_m)^\top \in \mathbb{C}^m \ \text{ with } \ \sum_{j=1}^{m} c_j = 0. \tag{2.7}$$

(iii) F is called positive semidefinite if for all $N \in \mathbb{N}$, $x_p \in \mathbb{R}^n$, $1 \leqslant p \leqslant N$, the matrix $(F(x_p - x_q))_{1\leqslant p,q\leqslant N} \in \mathbb{C}^{N\times N}$ is positive semidefinite.

(iv) F is called conditionally positive semidefinite if for all $N \in \mathbb{N}$, $x_p \in \mathbb{R}^n$, $1 \leqslant p \leqslant N$, the matrix $(F(x_p - x_q))_{1\leqslant p,q\leqslant N} \in \mathbb{C}^{N\times N}$ is conditionally positive semidefinite.

(v) Let $T \in \mathcal{B}\big(L^2(\mathbb{R}^n)\big)$. Then T is called positivity preserving $(in\ L^2(\mathbb{R}^n))$ if for any $0 \leqslant f \in L^2(\mathbb{R}^n)$ also $Tf \geqslant 0$.

In connection with Definition 2.1 (iv) one can show that if F is conditionally positive semidefinite, then (cf. [13, Lemma 2.5 (iii)], [20, p. 12])

$$F(-x) = \overline{F(x)}, \quad x \in \mathbb{R}^n. \tag{2.8}$$

In addition, one observes that for T to be positivity preserving it suffices to take $0 \leqslant f \in C_0^\infty(\mathbb{R}^n)$ in Definition 2.1 (v).

Given $F \in C(\mathbb{R}^n)$ and F polynomially bounded, one can define

$$F(-i\nabla)\colon \begin{cases} C_0^\infty(\mathbb{R}^n) \to L^2(\mathbb{R}^n), \\ f \mapsto F(-i\nabla)f = \big(f^\wedge F\big)^\vee. \end{cases} \tag{2.9}$$

More generally, if $F \in L^1_{\mathrm{loc}}(\mathbb{R}^n)$, one introduces the maximally defined operator of multiplication by F in $L^2(\mathbb{R}^n)$, denoted by M_F, by

$$(M_F f)(x) = F(x)f(x), \quad f \in \mathrm{dom}(M_F) = \big\{g \in L^2(\mathbb{R}^n) \,\big|\, Fg \in L^2(\mathbb{R}^n)\big\}, \tag{2.10}$$

and then defines $F(-i\nabla)$ as a normal operator in $L^2(\mathbb{R}^n)$ via

$$F(-i\nabla) = \mathcal{F}^{-1} M_F \mathcal{F} \tag{2.11}$$

(cf. (2.4), (2.5) and their unitary extensions to $L^2(\mathbb{R}^n)$).

Theorem 2.2 (cf., e.g., [15]**,** [18]**,** [21, Theorems XIII.52 and XIII.53]**,** [23]**).** *Assume that $F \in C(\mathbb{R}^n)$ and there exists $c \in \mathbb{R}$ such that $\mathrm{Re}(F(x)) \leqslant c$. Then the following items (i)–(iv) are equivalent:*

(i) *For all $t > 0$, $\exp(tF(-i\nabla))$ is positivity preserving in $L^2(\mathbb{R}^n)$.*

(ii) *For each $t > 0$, e^{tF} is a positive semidefinite function.*

(iii) *F is conditionally positive semidefinite.*

(iv) *(The Levy–Khintchine formula). There exist $\alpha \in \mathbb{R}$, $\beta \in \mathbb{R}^n$, $0 \leqslant A \in \mathbb{C}^{n\times n}$, and a nonnegative finite measure ν on $\mathbb{R}^n$, with $\nu(\{0\}) = 0$, such that*

$$\begin{aligned} F(x) &= \alpha + i(\beta, x)_{\mathbb{R}^n} - (x, Ax)_{\mathbb{C}^n} \\ &\quad + \int_{\mathbb{R}^n} \bigg[\exp(i(x,y)_{\mathbb{R}^n}) - 1 - \frac{i(x,y)_{\mathbb{R}^n}}{1 + \|y\|^2_{\mathbb{R}^n}}\bigg] \frac{1 + \|y\|^2_{\mathbb{R}^n}}{\|y\|^2_{\mathbb{R}^n}}\, d\nu(y), \quad x \in \mathbb{R}^n. \end{aligned} \tag{2.12}$$

Just for completeness (as it is used repeatedly in the bulk of this paper), we recall that item (ii) above implies item (iii) by differentiating $\exp_H\big(t(F(x_p - x_q))_{1\leqslant p,q\leqslant N}\big)$, $x_p \in \mathbb{R}^n$, $1 \leqslant p \leqslant N$, $N \in \mathbb{N}$, at $t = 0$. Conversely, that item (iii) implies item (ii) is a consequence of [16, Theorem 6.3.6].

We continue by recalling Bochner's classical theorem [7]:

Theorem 2.3 (Bochner's Theorem, cf., e.g., [2, Sect. 5.4]**,** [18, Theorem 2.7]**,** [20, p. 13]**,** [22, p. 46]**).** *Assume that $F \in C(\mathbb{R}^n)$. Then the following items (i) and (ii) are equivalent:*

(i) *F is positive semidefinite.*

(ii) *There exists a nonnegative finite measure μ on $\mathbb{R}^n$ such that*

$$F(x) = \mu^\wedge(x), \quad x \in \mathbb{R}^n. \tag{2.13}$$

In addition, if one of conditions (i) or (ii) holds, then

$$F(-x) = \overline{F(x)}, \quad |F(x)| \leqslant |F(0)|, \quad x \in \mathbb{R}^n, \tag{2.14}$$

in particular, F is bounded on $\mathbb{R}^n$.

Next, we turn to the finite-dimensional special case of an infinite-dimensional extension of Bochner's theorem in connection with locally compact Abelian groups due to Berberian [3] (see also [10, 11, 19, 24]):

Definition 2.4. *Let $F\colon \mathbb{R}^n \to \mathbb{C}^{m\times m}$, $m, n \in \mathbb{N}$. Then F is called positive semidefinite if for all $N \in \mathbb{N}$, $x_p \in \mathbb{R}^n$, $1 \leqslant p \leqslant N$, the block matrix $(F(x_p - x_q))_{1\leqslant p,q\leqslant N} \in \mathbb{C}^{mN\times mN}$ is nonnegative.*

Remark 2.5. By [13, Lemma 2.5 (i)], $F\colon \mathbb{R}^n \to \mathbb{C}^{m\times m}$ is positive semidefinite if and only if for all $N \in \mathbb{N}$, $x_p \in \mathbb{R}^n$, $c_p \in \mathbb{C}^m$, $1 \leqslant p \leqslant N$, one has

$$\sum_{p,q=1}^{N} (c_p, F(x_p - x_q)c_q)_{\mathbb{C}^m} \geqslant 0. \tag{2.15}$$

Theorem 2.6 ([3, p 178, Theorem 3 and Corollary on p. 177]**).**
Assume that $F \in C(\mathbb{R}^n, \mathbb{C}^{m\times m}) \cap L^\infty(\mathbb{R}^n, \mathbb{C}^{m\times m})$, $m \in \mathbb{N}$. Then the following items (i) and (ii) are equivalent:

(i) F is positive semidefinite.

(ii) There exists a nonnegative measure $\mu \in \mathcal{M}(\mathbb{R}^n, \mathbb{C}^{m\times m})$ such that

$$F(x) = \mu^\wedge(x), \quad x \in \mathbb{R}^n. \tag{2.16}$$

In addition, if one of conditions (i) or (ii) holds, then

$$F(-x) = F(x)^*, \quad \|F(x)\|_{\mathcal{B}(\mathbb{C}^m)} \leqslant \|F(0)\|_{\mathcal{B}(\mathbb{C}^m)}, \quad x \in \mathbb{R}^n. \tag{2.17}$$

Finally, we briefly turn to Fourier multipliers.

Definition 2.7. *Let $p, q \in [1,\infty) \cup \{\infty\}$. The set $\mathcal{M}^{p,q}(\mathbb{R}^n)$ denotes the Banach space of all bounded linear operators from $L^p(\mathbb{R}^n)$ to $L^q(\mathbb{R}^n)$ that commute with translations. The norm of $T \in \mathcal{M}^{p,q}(\mathbb{R}^n)$ is given by the operator norm,*

$$\|T\|_{p,q} := \|T\|_{\mathcal{B}(L^p(\mathbb{R}^n), L^q(\mathbb{R}^n))}. \tag{2.18}$$

We note that bounded convolution operators from $L^p(\mathbb{R}^n)$ to $L^q(\mathbb{R}^n)$ clearly are commuting with translations (i.e., are translation invariant); that the converse is valid as well is proved in [14, Theorem 2.5.2].

Given a complex measure μ on $\mathbb{R}^n$, the total variation of μ is defined by $|\mu|(\mathbb{R}^n)$ and the norm of μ is introduced as $\|\mu\| = |\mu|(\mathbb{R}^n)$. Given a μ-integrable $f\colon \mathbb{R}^n \to \mathbb{C}$, one defines the convolution of f and μ by

$$f * \mu\colon \begin{cases} \mathbb{R}^n \to \mathbb{C}, \\ x \mapsto (f * \mu)(x) = \int_{\mathbb{R}^n} f(x-y)\, d\mu(y), \end{cases} \quad x \in \mathbb{R}^n. \tag{2.19}$$

Also, one can introduce the associated convolution operator $T_\mu \in \mathcal{B}\big(L^p(\mathbb{R}^n)\big)$, $p \in [1,\infty)$, by

$$T_\mu f = f * \mu, \quad f \in L^p(\mathbb{R}^n). \tag{2.20}$$

Similarly, if $u \in \mathcal{S}'(\mathbb{R}^n)$ is a tempered distribution, the associated convolution operator T_u is defined via

$$T_u f = f * u, \quad f \in \mathcal{S}(\mathbb{R}^n). \tag{2.21}$$

In the cases $p = q = 1, 2$ one has the following well-known results:

Theorem 2.8 (cf., e.g., [14, Theorems 2.5.8 and 2.5.10]**).**
(i) $T \in \mathcal{M}^{1,1}(\mathbb{R}^n)$ if and only if $T = T_\mu$ for some (finite) complex measure μ. In this case

$$\|T\|_{1,1} = \|T_\mu\|_{\mathcal{B}(L^1(\mathbb{R}^n))} = |\mu|(\mathbb{R}^n). \tag{2.22}$$

(ii) $T \in \mathcal{M}^{2,2}(\mathbb{R}^n)$ if and only if $T = T_u$ for some $u \in \mathcal{S}'(\mathbb{R}^n)$, whose Fourier transform $u^\wedge$ lies in $L^\infty(\mathbb{R}^n)$. In this case

$$\|T\|_{2,2} = \|T_u\|_{\mathcal{B}(L^2(\mathbb{R}^n))} = \big\|u^\wedge\big\|_{L^\infty(\mathbb{R}^n)}. \tag{2.23}$$

3. On Positivity Preserving Linear Operators in $L^p(\mathbb{R}^n)^m$

In our principal section we now characterize linear, positivity preserving, translation invariant operators in $L^p(\mathbb{R}^n)^m$, $p \in [1, \infty)$, $m, n \in \mathbb{N}$.

We start with the following result:

Lemma 3.1. *Let $n \in \mathbb{N}$, and suppose that $F_\ell \colon \mathbb{R}^n \to \mathbb{C}$, $\ell = 1, 2$, are positive semidefinite. Then $F_1 F_2 : \mathbb{R}^n \to \mathbb{C}$ is positive semidefinite.*

Proof. Let $N \in \mathbb{N}$, $x_p \in \mathbb{R}^n$, $1 \leqslant p \leqslant N$, then by hypothesis,

$$(F_\ell(x_p - x_q))_{1 \leqslant p,q \leqslant N} \geqslant 0, \quad \ell = 1, 2,$$

and hence by Schur's theorem (see, e.g., the Lemma in [21, p. 215]),

$$((F_1F_2)(x_p - x_q))_{1 \leqslant p,q \leqslant N} = (F_1(x_p - x_q))_{1 \leqslant p,q \leqslant N} \circ_H (F_2(x_p - x_q))_{1 \leqslant p,q \leqslant N} \geqslant 0. \tag{3.1}$$

Here $A \circ_H B$ denotes the *Hadamard product* of two matrices $A, B \in \mathbb{C}^{N\times N}$, defined by

$$(A \circ_H B)_{j,k} = A_{j,k} B_{j,k}, \quad 1 \leqslant j, k \leqslant N. \tag{3.2}$$

□

The principal result on positivity preserving, translation invariant, linear operators in $L^p(\mathbb{R}^n)^m$, $p \in [1, \infty)$, $m, n \in \mathbb{N}$, proved in this note then reads as follows:

Theorem 3.2. *Let $m, n \in \mathbb{N}$, and $G \colon \mathbb{R}^n \to \mathbb{C}^{m\times m}$ be bounded and continuous. Then the following items (i)–(iv) are equivalent:*

(i) For all $1 \leqslant j, k \leqslant m$, $G_{j,k} \colon \mathbb{R}^n \to \mathbb{C}$ is positive semidefinite.

(ii) The linear operator,

$$G(-i\nabla)\big|_{C_0^\infty(\mathbb{R}^n)^m} : \begin{cases} C_0^\infty(\mathbb{R}^n)^m \to C_\infty(\mathbb{R}^n)^m, \\ (f_1, \dots, f_m)^\top \mapsto \Big(G\big(f_1^\wedge, \dots, f_m^\wedge\big)^\top\Big)^\vee, \end{cases} \tag{3.3}$$

extends boundedly to $G(-i\nabla) \in \mathcal{B}\big(L^1(\mathbb{R}^n)^m\big)$ *satisfying*

$$G(-i\nabla)\big(L^1(\mathbb{R}^n)_+^m\big) \subseteq L^1(\mathbb{R}^n)_+^m. \tag{3.4}$$

(*iii*) *There exists* $p \in (1,\infty)$ *such that the linear operator* (3.3) *extends boundedly to* $G(-i\nabla) \in \mathcal{B}\big(L^p(\mathbb{R}^n)^m\big)$ *satisfying*

$$G(-i\nabla)\big(L^p(\mathbb{R}^n)_+^m\big) \subseteq L^p(\mathbb{R}^n)_+^m. \tag{3.5}$$

(*iv*) *For all* $p \in (1,\infty)$, *the linear operator* (3.3) *extends boundedly to* $G(-i\nabla) \in \mathcal{B}\big(L^p(\mathbb{R}^n)^m\big)$ *satisfying*

$$G(-i\nabla)\big(L^p(\mathbb{R}^n)_+^m\big) \subseteq L^p(\mathbb{R}^n)_+^m. \tag{3.6}$$

Proof. We begin by proving the equivalence of items (*i*) and (*ii*).

First, suppose (*i*) holds. By Bochner's theorem (cf. Theorem 2.3), there exist finite, nonnegative Borel measures $\mu_{j,k}$ on $\mathbb{R}^n$ such that $G_{j,k} = \mu_{j,k}^\wedge$, $1 \leqslant j,k \leqslant m$. Thus, the classical $L^1(\mathbb{R}^n)$-multiplier theorem (cf. Theorem 2.8 (*i*)) implies that $G_{j,k}(-i\nabla)$ is an $L^1(\mathbb{R}^n)$-multiplier operator for all $1 \leqslant j,k \leqslant m$, that is, $G_{j,k}(-i\nabla) \in \mathcal{M}^{1,1}(\mathbb{R}^n)$, $1 \leqslant j,k \leqslant m$. With $\|G_{j,k}(-i\nabla)\|_{1,1}$ denoting the operator norm of $G_{j,k}(-i\nabla)$ in $L^1(\mathbb{R}^n)$, $1 \leqslant j,k \leqslant m$, we introduce

$$\|G(-i\nabla)\|_{1,1} := \max_{1\leqslant j,k\leqslant m} \{\|G_{j,k}(-i\nabla)\|_{1,1}\}. \tag{3.7}$$

Then, for $f = (f_1,\dots,f_m)^\top \in C_0^\infty(\mathbb{R}^n)^m$,

$$\big\|\big[G(-i\nabla)\big|_{C_0^\infty(\mathbb{R}^n)^m} f\big]_j\big\|_{L^1(\mathbb{R}^n)} \leqslant \|G(-i\nabla)\|_{1,1}\|f\|_{L^1(\mathbb{R}^n)^m}, \quad 1 \leqslant j \leqslant m, \tag{3.8}$$

and hence,

$$\big\|G(-i\nabla)\big|_{C_0^\infty(\mathbb{R}^n)^m} f\big\|_{L^1(\mathbb{R}^n)^m} \leqslant m\|G(-i\nabla)\|_{1,1}\|f\|_{L^1(\mathbb{R}^n)^m}. \tag{3.9}$$

In other words, $G(-i\nabla)\big|_{C_0^\infty(\mathbb{R}^n)^m}$ extends boundedly to an operator $G(-i\nabla) \in \mathcal{B}\big(L^1(\mathbb{R}^n)^m\big)$.

Since by [1, Theorem 2.29 (c)], $C_0^\infty(\mathbb{R}^n)_+^m$ is dense in $L^1(\mathbb{R}^n)_+^m$, to show that item (*ii*) holds, it suffices to prove that

$$G(-i\nabla)\big(C_0^\infty(\mathbb{R}^n)_+^m\big) \subseteq L^1(\mathbb{R}^n)_+^m. \tag{3.10}$$

Let $f = (f_1,\dots,f_m)^\top \in C_0^\infty(\mathbb{R}^n)_+^m$. By Bochner's theorem (cf. Theorem 2.3, with measures of the form $\mu_j = f_j d^n x$, $1 \leqslant j \leqslant m$), $f_k^\wedge$, $1 \leqslant k \leqslant m$, are positive semidefinite, and thus an application of Lemma 3.1 yields that $\sum_{k=1}^m G_{j,k} f_k^\wedge$, $1 \leqslant j \leqslant m$, are positive semidefinite. Since

$$([G(-i\nabla)f]_j)^\wedge = \sum_{k=1}^m G_{j,k} f_k^\wedge, \quad 1 \leqslant j \leqslant m, \tag{3.11}$$

applying Bochner's theorem once more implies that $[G(-i\nabla)f]_j \geqslant 0$, $1 \leqslant j \leqslant m$, that is,

$$G(-i\nabla)f \in L^1(\mathbb{R}^n)_+^m. \tag{3.12}$$

Thus, item (*ii*) holds.

Next, we assume that item (ii) holds. Let $\varphi\colon [0,\infty) \to [0,\infty)$ satisfy

$$\begin{aligned}&(\alpha)\ \varphi(\,\cdot\,) \text{ is decreasing on } [0,\infty),\\ &(\beta)\ \varphi \in C^\infty([0,\infty)), \quad \varphi^{(k)}(0) = 0,\ k \in \mathbb{N}, \quad \operatorname{supp}(\varphi) = [0,1],\\ &(\gamma)\ \int_{\mathbb{R}^n} d^n x\, \phi(x) = 1, \quad \phi(x) = \varphi(\|x\|_{\mathbb{R}^n}),\ x \in \mathbb{R}^n,\end{aligned} \tag{3.13}$$

and introduce

$$\phi_\varepsilon(x) = \varepsilon^{-n}\phi(x/\varepsilon), \quad \varepsilon \in (0,1),\ x \in \mathbb{R}^n, \tag{3.14}$$

implying

$$\lim_{\varepsilon\downarrow 0} \phi_\varepsilon^\wedge(\xi) = 1, \quad \xi \in \mathbb{R}^n. \tag{3.15}$$

Moreover we introduce

$$\phi_{\varepsilon,k} \in L^1(\mathbb{R}^n)_+^m, \quad [\phi_{\varepsilon,k}]_j = \begin{cases} 0, & j \neq k, \\ \phi_\varepsilon, & j = k, \end{cases} \quad 1 \leqslant j,k \leqslant m,\ \varepsilon \in (0,1). \tag{3.16}$$

Then by hypothesis,

$$G(-i\nabla)\phi_{\varepsilon,k} = \Big(\big(G_{1,k}\phi_\varepsilon^\wedge\big)^\vee, \dots, \big(G_{m,k}\phi_\varepsilon^\wedge\big)^\vee\Big)^\top \in L^1(\mathbb{R}^n)_+^m, \tag{3.17}$$

and hence, once more by Bochner's theorem, $G_{j,k}\phi_\varepsilon^\wedge$, $1 \leqslant j,k \leqslant m$, are positive semidefinite. Thus, for all $x_p \in \mathbb{R}^n$, $1 \leqslant p \leqslant N$, (3.15) implies

$$0 \leqslant \lim_{\varepsilon\downarrow 0} \big(G_{j,k}(x_p - x_q)\phi_\varepsilon^\wedge(x_p - x_q)\big)_{1\leqslant p,q\leqslant N} = (G_{j,k}(x_p - x_q))_{1\leqslant p,q\leqslant N}, \tag{3.18}$$

that is, $G_{j,k}$, $1 \leqslant j,k \leqslant m$, are positive semidefinite, implying item (i).

Next we prove that item (ii) implies item (iv). Assuming item (ii) holds, then by the equivalence of items (i) and (ii) just proved, $G_{j,k}$, $1 \leqslant j,k \leqslant m$, are positive semidefinite and hence there exist finite, nonnegative Borel measures $\mu_{j,k}$ on $\mathbb{R}^n$, such that $G_{j,k} = \mu_{j,k}^\wedge$, $1 \leqslant j,k \leqslant m$. By the classical L^1-multiplier theorem (cf. Theorem 2.8 (i)), this implies that $G_{j,k}(-i\nabla)$, $1 \leqslant j,k \leqslant m$, are $L^1(\mathbb{R}^n)$-multiplier operators, and hence also $L^p(\mathbb{R}^n)$-multipliers for all $p \in [1,\infty)$ according to [14, p. 143, remarks after Definition 2.5.11]. We denote by $\|G_{j,k}(-i\nabla)\|_{p,p}$ the norm of $G_{j,k}(-i\nabla)$ in $L^p(\mathbb{R}^n)$, $1 \leqslant j,k \leqslant m$, $p \in (1,\infty)$, and introduce

$$\|G(-i\nabla)\|_{p,p} := \max_{1\leqslant j,k\leqslant m}\{\|G_{j,k}(-i\nabla)\|_{p,p}\}. \tag{3.19}$$

Then for all $f = (f_1,\dots,f_m)^\top \in C_0^\infty(\mathbb{R}^n)^m$,

$$\big\|G(-i\nabla)\big|_{C_0^\infty(\mathbb{R}^n)^m} f\big\|_{L^p(\mathbb{R}^n)^m} \leqslant m\|G(-i\nabla)\|_{p,p}\|f\|_{L^p(\mathbb{R}^n)^m}, \tag{3.20}$$

and thus $G(-i\nabla)\big|_{C_0^\infty(\mathbb{R}^n)^m}$ can be extended to a bounded operator $G(-i\nabla) \in \mathcal{B}\big(L^p(\mathbb{R}^n)^m\big)$.

Since once more by [1, Theorem 2.29 (c)], $C_0^\infty(\mathbb{R}^n)_+^m$ is dense in $L^p(\mathbb{R}^n)_+^m$, $p \in [1,\infty)$, to show that item (iv) is valid it suffices to prove that

$$[G(-i\nabla)f]_j \geqslant 0, \quad 1 \leqslant j \leqslant m,\ f = (f_1,\dots,f_m)^\top \in C_0^\infty(\mathbb{R}^n)_+^m, \tag{3.21}$$

which is implied by item (ii).

It is clear that item (*iv*) implies item (*iii*).

Next, we prove that item (*iii*) implies item (*i*). We start by proving that for all $f = (f_1, \dots, f_m)^\top \in C_0^\infty(\mathbb{R}^n)_+^m$, and all $1 \leqslant j \leqslant m$, $\sum_{k=1}^m G_{j,k} f_k^\wedge$ is positive semidefinite. Since $G(\,\cdot\,)$ is bounded, the map

$$f \mapsto G(-i\nabla)f = \big(Gf^\wedge\big)^\vee, \quad f \in C_0^\infty(\mathbb{R}^n)^m, \tag{3.22}$$

extends to a bounded operator in $\mathcal{B}\big(L^2(\mathbb{R}^n)^m\big)$ by the classical L^2-multiplier theorem, Theorem 2.8 (*ii*). Thus, for all $R > 0$, $f = (f_1, \dots, f_m)^\top \in C_0^\infty(\mathbb{R}^n)_+^m$, and for all $1 \leqslant j \leqslant m$, $[G(-i\nabla)f]_j \chi_{B_n(0,R)} \in L^1(\mathbb{R}^n)_+ \cap L^2(\mathbb{R}^n)_+$. Thus, again by Bochner's theorem, $([G(-i\nabla)f]_j \chi_{B_n(0,R)})^\wedge$, $1 \leqslant j \leqslant m$, are positive semidefinite. Hence, taking limits in $L^2(\mathbb{R}^n)$, one obtains,

$$\sum_{k=1}^m G_{j,k} f_k^\wedge = ([G(-i\nabla)f]_j)^\wedge = \lim_{R\uparrow\infty} ([G(-i\nabla)f]_j \chi_{B_n(0,R)})^\wedge, \tag{3.23}$$

and thus there exist a sequence of increasing positive numbers $\{R_\ell\}_{\ell\in\mathbb{N}}$, with $\lim_{\ell\to\infty} R_\ell = \infty$, and a set $E \subset \mathbb{R}^n$ of Lebesgue measure zero, $|E| = 0$, such that for all $x \in \mathbb{R}^n \backslash E$,

$$\lim_{\ell\to\infty} ([G(-i\nabla)f]_j \chi_{B_n(0,R_\ell)})^\wedge(x) = \sum_{k=1}^m G_{j,k}(x) f_k^\wedge(x). \tag{3.24}$$

Letting $x_p \in \mathbb{R}^n$, $1 \leqslant p \leqslant N$, for each $1 \leqslant q \leqslant N$, one can choose a sequence $\{x_{q,r}\}_{r\in\mathbb{N}} \subset \mathbb{R}^n \backslash E$ such that $\lim_{r\to\infty} x_{q,r} = x_q$, $1 \leqslant q \leqslant N$, and that

$$(x_{p,r} - x_{q,r}) \in \mathbb{R}^n \backslash E, \quad 1 \leqslant p, q \leqslant N, \ r \in \mathbb{N}. \tag{3.25}$$

Hence, employing that $\sum_{k=1}^m G_{j,k} f_k^\wedge$, $1 \leqslant j \leqslant m$, is continuous, one concludes that

$$\begin{aligned} &\left(\sum_{k=1}^m G_{j,k}(x_p - x_q) f_k^\wedge(x_p - x_q)\right)_{1\leqslant p,q\leqslant N} \\ &\quad = \lim_{r\to\infty} \left(\sum_{k=1}^m G_{j,k}(x_{p,r} - x_{q,r}) f_k^\wedge(x_{p,r} - x_{q,r})\right)_{1\leqslant p,q\leqslant N} \\ &\quad = \lim_{r\to\infty} \lim_{\ell\to\infty} \big(([G(-i\nabla)f]_j \chi_{B_n(0,R_\ell)})^\wedge(x_{p,r} - x_{q,r})\big)_{1\leqslant p,q\leqslant N} \\ &\quad \geqslant 0, \end{aligned} \tag{3.26}$$

implying that $\sum_{k=1}^m G_{j,k} f_k^\wedge$, $1 \leqslant j \leqslant m$, are positive semidefinite. Next, introduce $\phi_{\varepsilon,k} \in C_0^\infty(\mathbb{R}^n)_+^m$, $1 \leqslant k \leqslant m$, $\varepsilon \in (0,1)$, as in (3.16). Then with $f = \phi_{\varepsilon,k}$, $1 \leqslant k \leqslant m$, $\varepsilon \in (0,1)$, in (3.26), one concludes that for all $\varepsilon \in (0,1)$, $1 \leqslant j,k \leqslant m$, $G_{j,k}\phi_\varepsilon^\wedge$ is positive semidefinite. Hence, again applying (3.15), one obtains that $G_{j,k} = \lim_{\varepsilon\downarrow 0} G_{j,k}\phi_\varepsilon^\wedge$ is positive semidefinite, and thus item (*i*) holds. ☐

Given $S \in \mathbb{C}^{m\times m}$, $m \in \mathbb{N}$, its *Hadamard exponential*, denoted by $\exp_H(S)$, is defined by

$$\exp_H(S) = \big(\exp_H(S)_{j,k} := \exp(S_{j,k})\big)_{1\leqslant j,k\leqslant m}. \tag{3.27}$$

More generally, if $S\colon \mathbb{R}^n \to \mathbb{C}^{m\times m}$, $m,n \in \mathbb{N}$, its *Hadamard exponential*, denoted by $\exp_H(S(\,\cdot\,))$, is defined by

$$\exp_H(S(x)) = \big(\exp_H(S(x))_{j,k} := \exp(S(x)_{j,k})\big)_{1\leqslant j,k\leqslant m}, \quad x \in \mathbb{R}^n. \tag{3.28}$$

Corollary 3.3. *Let $m,n \in \mathbb{N}$, suppose that $F\colon \mathbb{R}^n \to \mathbb{C}^{m\times m}$ is continuous, and assume there exists $c \in \mathbb{R}$ such that*

$$\operatorname{Re}(F_{j,k}) \leqslant c, \quad 1 \leqslant j,k \leqslant m. \tag{3.29}$$

Then the following items (i)–(vi) are equivalent:

(i) *There exists $p \in (1,\infty)$ such that for all $t > 0$, the linear operator*

$$(\exp_H(tF))(-i\nabla)\big|_{C_0^\infty(\mathbb{R}^n)^m}\colon \begin{cases} C_0^\infty(\mathbb{R}^n)^m \to C_\infty(\mathbb{R}^n)^m, \\ (f_1,\dots,f_m)^\top \mapsto \Big(\exp_H(tF)\big(f_1^\wedge,\dots,f_m^\wedge\big)^\top\Big)^\vee, \end{cases} \tag{3.30}$$

extends to a bounded operator $(\exp_H(tF))(-i\nabla) \in \mathcal{B}\big(L^p(\mathbb{R}^n)^m\big)$ satisfying

$$(\exp_H(tF))(-i\nabla)\big(L^p(\mathbb{R}^n)_+^m\big) \subseteq L^p(\mathbb{R}^n)_+^m. \tag{3.31}$$

(ii) *For all $p \in (1,\infty)$, and all $t > 0$, the linear operator* (3.30) *extends boundedly to $(\exp_H(tF))(-i\nabla) \in \mathcal{B}\big(L^p(\mathbb{R}^n)^m\big)$ satisfying*

$$(\exp_H(tF))(-i\nabla)\big(L^p(\mathbb{R}^n)_+^m\big) \subseteq L^p(\mathbb{R}^n)_+^m. \tag{3.32}$$

(iii) *For all $t > 0$, the linear operator* (3.30) *extends boundedly to $(\exp_H(tF))(-i\nabla) \in \mathcal{B}\big(L^1(\mathbb{R}^n)^m\big)$ satisfying*

$$(\exp_H(tF))(-i\nabla)\big(L^1(\mathbb{R}^n)_+^m\big) \subseteq L^1(\mathbb{R}^n)_+^m. \tag{3.33}$$

(iv) *For all $1 \leqslant j,k \leqslant m$, and all $t > 0$, $\exp(tF_{j,k})\colon \mathbb{R}^n \to \mathbb{C}$ is positive semidefinite.*

(v) *For all $1 \leqslant j,k \leqslant m$, $F_{j,k}\colon \mathbb{R}^n \to \mathbb{C}$ is conditionally positive semidefinite.*

(vi) *For all $1 \leqslant j,k \leqslant m$, there exist $\alpha_{j,k} \in \mathbb{R}$, $\beta_{j,k} \in \mathbb{R}^n$, $0 \leqslant A(j,k) \in \mathbb{C}^{n\times n}$, and a nonnegative, finite Borel measure $\nu_{j,k}$ on $\mathbb{R}^n$, satisfying $\nu_{j,k}(\{0\}) = 0$, such that*

$$\begin{aligned} F_{j,k}(x) &= \alpha_{j,k} + i(\beta_{j,k},x)_{\mathbb{R}^n} - (x,A(j,k)x)_{\mathbb{C}^n} \\ &\quad + \int_{\mathbb{R}^n} \bigg[\exp(i(x,y)_{\mathbb{R}^n}) - 1 - \frac{i(x,y)_{\mathbb{R}^n}}{1+\|y\|_{\mathbb{R}^n}^2}\bigg] \frac{1+\|y\|_{\mathbb{R}^n}^2}{\|y\|_{\mathbb{R}^n}^2}\, d\nu_{j,k}(y), \quad x \in \mathbb{R}^n. \end{aligned} \tag{3.34}$$

Proof. The equivalence of items (iv), (v), and (vi) follows from classical results (cf. [21, Theorems XIII.52 and XIII.53]). The equivalence of items (i), (ii), (iii), and (iv) follows from Theorem 3.2, putting $G = \exp_H(tF)$, $t > 0$. ☐

Corollary 3.4. *Let $m,n \in \mathbb{N}$, suppose that $F\colon \mathbb{R}^n \to \mathbb{C}^{m\times m}$ is a continuous, diagonal, matrix-valued function, and assume there exists $c \in \mathbb{R}$ such that*

$$\operatorname{Re}(F_{j,j}) \leqslant c, \quad 1 \leqslant j \leqslant m. \tag{3.35}$$

Then the following items (i)–(iv) are equivalent:

(i) For all $1 \leqslant j \leqslant m$, *$F_{j,j}$ is conditionally positive semidefinite.*

(ii) For all $t > 0$, the linear operator

$$(\exp(tF))(-i\nabla)\big|_{C_0^\infty(\mathbb{R}^n)^m} : \begin{cases} C_0^\infty(\mathbb{R}^n)^m \to C_\infty(\mathbb{R}^n)^m, \\ (f_1, \dots, f_m)^\top \mapsto \Big(\exp(tF)\big(f_1^\wedge, \dots, f_m^\wedge\big)^\top\Big)^\vee, \end{cases} \tag{3.36}$$

extends boundedly to $(\exp(tF))(-i\nabla) \in \mathcal{B}\big(L^1(\mathbb{R}^n)^m\big)$ *satisfying*

$$(\exp(tF))(-i\nabla)\big(L^1(\mathbb{R}^n)_+^m\big) \subseteq L^1(\mathbb{R}^n)_+^m. \tag{3.37}$$

(iii) There exists $p \in (1, \infty)$ such that for all $t > 0$, the linear operator (3.36) *extends boundedly to* $(\exp(tF))(-i\nabla) \in \mathcal{B}\big(L^p(\mathbb{R}^n)^m\big)$ *satisfying*

$$(\exp(tF))(-i\nabla)\big(L^p(\mathbb{R}^n)_+^m\big) \subseteq L^p(\mathbb{R}^n)_+^m. \tag{3.38}$$

(iv) For all $p \in (1, \infty)$, and all $t > 0$, the linear operator (3.36) *extends boundedly to* $(\exp(tF))(-i\nabla) \in \mathcal{B}\big(L^p(\mathbb{R}^n)^m\big)$ *satisfying*

$$(\exp(tF))(-i\nabla)\big(L^p(\mathbb{R}^n)_+^m\big) \subseteq L^p(\mathbb{R}^n)_+^m. \tag{3.39}$$

Proof. By the assumptions on F, $\exp(tF)\colon \mathbb{R}^n \to \mathbb{C}^{m\times m}$ is a bounded, continuous, diagonal, matrix-valued function whose diagonal entries are

$$\exp(tF)_{j,j} = \exp(tF_{j,j}), \quad t > 0,\ 1 \leqslant j \leqslant m. \tag{3.40}$$

By Theorem 3.2, with $G = \exp(tF)$, $t > 0$, it suffices to prove that item (i) is equivalent to

$(i)(\alpha)$ For all $1 \leqslant j, k \leqslant m$, and all $t > 0$, $\exp(tF)_{j,k}\colon \mathbb{R}^n \to \mathbb{C}$ is positive semidefinite.

Since $\exp(tF)$ is a diagonal matrix, item $(i)(\alpha)$ is equivalent to

$(i)(\beta)$ For all $1 \leqslant j \leqslant m$, and all $t > 0$, $\exp(tF)_{j,j} = \exp(tF_{j,j})$ is positive semidefinite.

However, the equivalence of items (i) and $(i)(\beta)$ follows from the equivalence of items (ii) and (iii) in Theorem 2.2. ☐

Corollary 3.5. *Let $m, n \in \mathbb{N}$, and assume that $F\colon \mathbb{R}^n \to \mathbb{C}^{m\times m}$ is bounded and continuous. Suppose that for all $1 \leqslant j, k \leqslant m$, $F_{j,k}\colon \mathbb{R}^n \to \mathbb{C}$ is positive semidefinite. Then for all $p \in [1, \infty)$, and all $t > 0$, the linear operator*

$$(\exp(tF))(-i\nabla)\big|_{C_0^\infty(\mathbb{R}^n)^m} : \begin{cases} C_0^\infty(\mathbb{R}^n)^m \to C_\infty(\mathbb{R}^n)^m, \\ (f_1, \dots, f_m)^\top \mapsto \Big(\exp(tF)\big(f_1^\wedge, \dots, f_m^\wedge\big)^\top\Big)^\vee, \end{cases} \tag{3.41}$$

extends boundedly to $(\exp(tF))(-i\nabla) \in \mathcal{B}\big(L^p(\mathbb{R}^n)^m\big)$ *satisfying*

$$(\exp(tF))(-i\nabla)\big(L^p(\mathbb{R}^n)_+^m\big) \subseteq L^p(\mathbb{R}^n)_+^m. \tag{3.42}$$

Proof. By the hypotheses on F, $\exp(tF)\colon \mathbb{R}^n \to \mathbb{C}^{m\times m}$ is bounded and continuous for all $t > 0$. By Theorem 3.2, with $G = \exp(tF)$, $t > 0$, it suffices to prove that for all $1 \leqslant j,k \leqslant m$ and all $t > 0$, $\exp(tF)_{j,k}\colon \mathbb{R}^n \to \mathbb{C}$ is positive semidefinite. Combining Lemma 3.1 with an induction argument shows that $\big(F^\ell\big)_{j,k}\colon \mathbb{R}^n \to \mathbb{C}$ is positive semidefinite for all $\ell \in \mathbb{N}$ and all $1 \leqslant j,k \leqslant m$. Thus, also $\exp(tF)_{j,k} = \sum_{\ell=0}^\infty \frac{t^\ell}{\ell!}(F^\ell)_{j,k}$ is positive semidefinite for all $t > 0$ and all $1 \leqslant j,k \leqslant m$. ☐

We conclude with an explicit illustration:

Example 3.6. Let $n \in \mathbb{N}$, assume that $a\colon \mathbb{R}^n \to \mathbb{R}$ is continuous and bounded above, $b \geqslant 0$ is constant, and define $F_0\colon \mathbb{R}^n \to \mathbb{C}^{2\times 2}$ by

$$F_0(x) = \begin{pmatrix} a(x) & b \\ b & a(x) \end{pmatrix}, \quad x \in \mathbb{R}^n. \tag{3.43}$$

Then the following items (i)–(iv) are equivalent:

(i) a is conditionally positive semidefinite.

(ii) F_0 is conditionally positive semidefinite in the sense of Mlak [19], that is, for all $N \in \mathbb{N}$, all $x_p \in \mathbb{R}^n$, and all $c_p \in \mathbb{C}^2$, $1 \leqslant p \leqslant N$, satisfying $\sum_{p=1}^N c_p = 0$, one has,

$$\sum_{p,q=1}^N (c_p, F_0(x_p - x_q)c_q)_{\mathbb{C}^2} \geqslant 0. \tag{3.44}$$

(iii) For all $t > 0$, $\exp(tF_0)\colon \mathbb{R}^n \to \mathbb{R}^{2\times 2}$ is positive semidefinite in the sense of [13, Definition 2.4] (cf. Definition 2.4).

(iv) For all $t > 0$, the linear operator

$$(\exp(tF_0))(-i\nabla)\big|_{C_0^\infty(\mathbb{R}^n)^m}\colon \begin{cases} C_0^\infty(\mathbb{R}^n)^m \to C_\infty(\mathbb{R}^n)^m, \\ (f_1,\dots,f_m)^\top \mapsto \Big(\exp(tF_0)\big(f_1^\wedge,\dots,f_m^\wedge\big)^\top\Big)^\vee, \end{cases} \tag{3.45}$$

extends boundedly to $(\exp(tF_0))(-i\nabla) \in \mathcal{B}\big(L^1(\mathbb{R}^n)^m\big)$ satisfying

$$(\exp(tF_0))(-i\nabla)\big(L^1(\mathbb{R}^n)_+^m\big) \subseteq L^1(\mathbb{R}^n)_+^m. \tag{3.46}$$

(v) There exists $p \in (1,\infty)$ such that for all $t > 0$, the linear operator (3.45) extends boundedly to $(\exp(tF_0))(-i\nabla) \in \mathcal{B}\big(L^p(\mathbb{R}^n)^m\big)$ satisfying

$$(\exp(tF_0))(-i\nabla)\big(L^p(\mathbb{R}^n)_+^m\big) \subseteq L^p(\mathbb{R}^n)_+^m. \tag{3.47}$$

(vi) For all $p \in (1,\infty)$, and all $t > 0$, the linear operator (3.45) extends boundedly to $(\exp(tF_0))(-i\nabla) \in \mathcal{B}\big(L^p(\mathbb{R}^n)^m\big)$ satisfying

$$(\exp(tF_0))(-i\nabla)\big(L^p(\mathbb{R}^n)_+^m\big) \subseteq L^p(\mathbb{R}^n)_+^m. \tag{3.48}$$

Proof. We start by proving the equivalence of items (i) and (ii). One notes that for $c_p = (c_{p,1}, c_{p,2})^\top \in \mathbb{C}^2$, $1 \leqslant p \leqslant N$, $N \in \mathbb{N}$,

$$\sum_{p,q=1}^{N} (c_p, F_0(x_p - x_q)c_q)_{\mathbb{C}^2} = \sum_{p,q=1}^{N} \overline{c_{p,1}}\, a(x_p - x_q)c_{q,1} + \sum_{p,q=1}^{N} \overline{c_{p,2}}\, a(x_p - x_q)c_{q,2} + b\bigg[\bigg(\sum_{p=1}^{N} \overline{c_{p,1}}\bigg)\bigg(\sum_{q=1}^{N} c_{q,2}\bigg) + \bigg(\sum_{p=1}^{N} \overline{c_{p,2}}\bigg)\bigg(\sum_{q=1}^{N} c_{q,1}\bigg)\bigg]. \tag{3.49}$$

If item (i) holds, then for $c_p = (c_{p,1}, c_{p,2})^\top \in \mathbb{C}^2$, $1 \leqslant p \leqslant N$, with $\sum_{p=1}^{N} c_p = 0$, (3.49) implies

$$\sum_{p,q=1}^{N} (c_p, F_0(x_p - x_q)c_q)_{\mathbb{C}^2} = \sum_{p,q=1}^{N} \overline{c_{p,1}}\, a(x_p - x_q)c_{q,1} + \sum_{p,q=1}^{N} \overline{c_{p,2}}\, a(x_p - x_q)c_{q,2} \geqslant 0, \tag{3.50}$$

implying item (ii).

Next, suppose item (ii) holds. Choose $d_p \in \mathbb{C}$, $1 \leqslant p \leqslant N$, $N \in \mathbb{N}$, with $\sum_{p=1}^{N} d_p = 0$. Let $c_p = (c_{p,1}, c_{p,2})^\top \in \mathbb{C}^2$, $1 \leqslant p \leqslant N$, be defined via

$$c_{p,1} = d_p, \quad c_{p,2} = 0, \quad 1 \leqslant p \leqslant N. \tag{3.51}$$

Then $\sum_{p=1}^{N} c_p = 0$ and (3.49) yields

$$0 \leqslant \sum_{p,q=1}^{N} (c_p, F_0(x_p - x_q)c_q)_{\mathbb{C}^2} = \sum_{p,q=1}^{N} \overline{d_p}\, a(x_p - x_q)d_q, \tag{3.52}$$

implying item (i).

Next we employ the elementary matrix identity

$$\exp\left(\begin{pmatrix} \alpha & \beta \\ \beta & \alpha \end{pmatrix}\right) = e^{\alpha} \begin{pmatrix} \cosh(\beta) & \sinh(\beta) \\ \sinh(\beta) & \cosh(\beta) \end{pmatrix}, \quad \alpha, \beta \in \mathbb{R}. \tag{3.53}$$

Then, if $b = 0$, the equivalence of items (i), (iv), (v), and (vi) follows from Corollary 3.4.

Next, suppose item (i) holds and that $b = 0$. We will show that then also item (iii) holds: Let $x_p \in \mathbb{R}^n$, and let $c_p = (c_{p,1}, c_{p,2})^\top \in \mathbb{C}^2$, $1 \leqslant p \leqslant N$, $N \in \mathbb{N}$. Then

$$\exp(tF_0)(x) = \begin{pmatrix} e^{ta(x)} & 0 \\ 0 & e^{ta(x)} \end{pmatrix}, \quad t > 0,\ x \in \mathbb{R}^n, \tag{3.54}$$

and hence by the equivalence of items (*ii*) and (*iii*) in Theorem 2.2,

$$\begin{aligned}\sum_{p,q=1}^{N} &(c_p, \exp(tF_0)(x_p - x_q)c_q)_{\mathbb{C}^2} \\ &= \sum_{p,q=1}^{N} \overline{c_{p,1}}\, e^{ta(x_p-x_q)} c_{q,1} + \sum_{p,q=1}^{N} \overline{c_{p,2}}\, e^{ta(x_p-x_q)} c_{q,2} \geqslant 0.\end{aligned} \tag{3.55}$$

Hence, item (*iii*) follows from [13, Lemma 2.5 (*i*)] (cf. Remark 2.5).

Now suppose item (*iii*) holds and that $b = 0$. We will show that then also item (*ii*) holds: Let $x_p \in \mathbb{R}^n$, and let $c_p \in \mathbb{C}^2$, $1 \leqslant p \leqslant N$, $N \in \mathbb{N}$, with $\sum_{p=1}^{N} c_p = 0$. Then (with I_2 the identity matrix in $\mathbb{C}^{2\times 2}$),

$$\begin{aligned} 0 &\leqslant \lim_{t\downarrow 0} t^{-1}\big(c_p, \exp(tF_0)(x_p - x_q)c_q\big)_{\mathbb{C}^2} \\ &= \lim_{t\downarrow 0} \sum_{p,q=1}^{N} \big(c_p, t^{-1}\big[\exp(tF_0)(x_p - x_q) - I_2\big]c_q\big)_{\mathbb{C}^2} \\ &= \sum_{p,q=1}^{N} (c_p, F_0(x_p - x_q)c_q)_{\mathbb{C}^2}, \end{aligned} \tag{3.56}$$

and hence items (*i*)–(*vi*) are equivalent if $b = 0$.

In the remainder of the proof we suppose that $b \neq 0$. We start by proving that item (*i*) implies item (*iii*). By inspection, the following matrix is nonnegative,

$$\begin{pmatrix} \cosh(tb) & \sinh(tb) \\ \sinh(tb) & \cosh(tb) \end{pmatrix} \geqslant 0, \tag{3.57}$$

as its eigenvalues $\cosh(tb) \pm \sinh(tb)$ are nonnegative. By item (*i*) and the equivalence of items (*ii*) and (*iii*) in Theorem 2.2, as well as Bochner's theorem, Theorem 2.3, for all $t > 0$, there exists a finite, nonnegative Borel measure ν_t on $\mathbb{R}^n$ such that $e^{ta} = \nu_t^{\wedge}$. Thus, (3.53) implies

$$\exp(tF_0(x)) = e^{ta(x)} \begin{pmatrix} \cosh(tb) & \sinh(tb) \\ \sinh(tb) & \cosh(tb) \end{pmatrix} = \left(\begin{pmatrix} \cosh(tb) & \sinh(tb) \\ \sinh(tb) & \cosh(tb) \end{pmatrix} \nu_t \right)^{\wedge}, \tag{3.58}$$

that is, $\exp(tF_0(x))$ is the Fourier transform of a nonnegative, finite, $\mathbb{C}^{2\times 2}$-valued measure, and hence item (*iii*) follows from Berberian's matrix-valued extension of Bochner's theorem, Theorem 2.6.

To verify that item (*iii*) implies item (*ii*), one notes that (3.56) remains valid if $b \neq 0$.

By equation (3.58), for all $t > 0$, the entries of $\exp(tF_0)$ are either $e^{ta}\cosh(tb)$ or $e^{ta}\sinh(tb)$, and hence for all $1 \leqslant j, k \leqslant 2$, $\exp(tF_0(\,\cdot\,))_{j,k}$ is positive semidefinite if and only if $e^{ta(\,\cdot\,)}$ is, and thus, by the equivalence of items (*ii*) and (*iii*) in Theorem 2.2, if and only if $a(\,\cdot\,)$ is conditionally positive semidefinite. The equivalence of items (*i*), (*iv*)–(*vi*) now follows from Theorem 3.2. □

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The Distribution of Path Lengths On Directed Weighted Graphs

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To the memory of Boris Pavlov, a teacher, colleague and friend

Abstract. We consider directed weighted graphs and define various families of path counting functions. Our main results are explicit formulas for the main term of the asymptotic growth rate of these counting functions, under some irrationality assumptions on the lengths of all closed orbits on the graph. In addition we assign transition probabilities to such graphs and compute statistics of the corresponding random walks. Some examples and applications are reviewed.

1. Introduction and Main Results

Questions regarding the distribution of path lengths on directed weighted graphs are encountered in various fields of study of mathematics and physics. They arise naturally in dynamics and the study of closed orbits of suspensions of shifts of finite type, see among others [15, 16, 9, 4], and the more recent [12, 3].

Our motivations for counting paths on weighted graphs are diverse. The second author's motivation originates in the study of a model of mathematical quasicrystals which we call multiscale substitution tilings, and in the study of equidistribution of what is known as Kakutani's partitions, first described in [11]. The connection to problems concerning path counting on weighted graphs is introduced in Sect. 5.2. The third author's motivation is rooted in theoretical physics, specifically in the spectral properties of the Schrödinger operator for systems which are chaotic in the classical limit and for metric graphs [8]. Of particular relevance are studies of the distribution of delay (transit) times through chaotic scatterers such as, e.g., the scattering of ultra-short electromagnetic pulses by complex molecules, or traversing networks of transmission lines [1, 20].

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1.1. Counting paths in graphs

Let $G = (\mathcal{V}, \mathcal{E}, l)$ be a directed weighted metric graph with a set $\mathcal{V} = \{1, \ldots, n\}$ of vertices and a set $\mathcal{E}$ of edges. A positive weight is assigned to each edge $\alpha \in \mathcal{E}$, and we think of this weight as the length of α. For a path γ connecting two vertices in $\mathcal{V}$, the path metric l is defined to be the sum of the weights of the edges in γ. When considering paths which do not necessarily terminate at a vertex of G, the path metric is defined by $l(\gamma) = a$ if the path γ is isometric to $[0, a] \subset \mathbb{R}$. Throughout this paper G is assumed to be a strongly connected multigraph, that is, a graph which admits a path from every vertex $i \in \mathcal{V}$ to every vertex $j \in \mathcal{V}$, and loops and multiple edges are allowed.

We say that G is a graph of incommensurable orbits, or **incommensurable** for short, if there exist at least two closed paths in G of lengths a, b such that $a \notin \mathbb{Q}b$. This irrationality condition on the lengths of the edges is equivalent to the set of lengths of all closed orbits in G not being a uniformly discrete subset of $\mathbb{R}$. Indeed, if there exist two closed paths in G of lengths a, b such that $a \notin \mathbb{Q}b$, then by Dirichlet's approximation theorem for every $\varepsilon > 0$ there exist $p, q \in \mathbb{N}$ such that $|aq - pb| < \varepsilon$, and so the set of lengths of closed orbits in G is not uniformly discrete. Conversely, if the set of lengths of closed orbits is rationally dependent, then the finiteness of the graph implies that there is a finite set L of lengths for which the length of any closed orbit in G is a linear combination with integer coefficients of elements in L. It follows that the set of lengths of closed orbits in G is uniformly discrete.

Let $i, j \in \mathcal{V}$ be a pair of vertices in G, and assume that there are $k \geq 0$ edges $\alpha_1, \ldots, \alpha_k$ from i to j. The matrix valued function $M : \mathbb{C} \to M_n(\mathbb{C})$, which we call the graph matrix function of G, is defined by

$$M_{ij}(s) = e^{-s \cdot l(\alpha_1)} + \cdots + e^{-s \cdot l(\alpha_k)}$$

and $M_{ij}(s) = 0$ if i is not connected to j by an edge. Note that the restriction of M to $\mathbb{R}$ is real valued.

Theorem 1. *Let G be a strongly connected incommensurable graph. There exist a positive constant λ and a matrix $Q \in M_n(\mathbb{R})$ with positive entries such that*

(i) *The number of paths from $i \in \mathcal{V}$ to $j \in \mathcal{V}$ of length at most x grows as*

$$\frac{1}{\lambda} Q_{ij} e^{\lambda x} + o\left(e^{\lambda x}\right), \quad x \to \infty.$$

(ii) *Let $\alpha \in \mathcal{E}$ be an edge in G which originates in vertex $j \in \mathcal{V}$. The number of paths of length exactly x from some vertex i to a point on the edge α grows as*

$$\frac{1 - e^{-l(\alpha)\lambda}}{\lambda} Q_{ij} e^{\lambda x} + o\left(e^{\lambda x}\right), \quad x \to \infty.$$

The constant λ is the maximal real value for which the spectral radius of M is equal to 1, and

$$Q = Q(M(\lambda)) = \frac{\operatorname{adj}(I - M(\lambda))}{-\operatorname{tr}(\operatorname{adj}(I - M(\lambda)) \cdot M'(\lambda))}$$

where M' is the entry-wise derivative of M, and adj$A$ *is the adjugate or classical adjoint matrix of A, that is the transpose of its cofactor matrix.*

Example. Let G be the directed weighted graph which appears in Fig. 1.

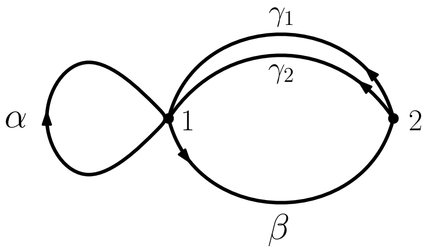

FIGURE 1. Graph with two vertices $\mathcal{V} = \{1, 2\}$ and four edges $\mathcal{E} = \{\alpha, \beta, \gamma_1, \gamma_2\}$.

The graph matrix function of G is given by

$$M(s) = \begin{pmatrix} e^{-l(\alpha)s} & e^{-l(\beta)s} \\ e^{-l(\gamma_1)s} + e^{-l(\gamma_2)s} & 0 \end{pmatrix}.$$

Putting, for example,

$$l(\alpha) = \log 2, \qquad l(\gamma_1) = \log \frac{3}{2},$$
$$l(\beta) = \log 2, \qquad l(\gamma_2) = \log 3,$$

we get $\lambda = 1$ and

$$Q = \frac{6}{\log 432} \begin{pmatrix} 1 & \frac{1}{2} \\ 1 & \frac{1}{2} \end{pmatrix},$$

and so by the second part of Theorem 1, the number of paths of length exactly x from vertex 1 to a point on the edge γ_2 grows as

$$\frac{1 - e^{-l(\gamma_2)\lambda}}{\lambda} Q_{12} e^{\lambda x} + o\left(e^{\lambda x}\right) = \frac{e^x}{\log \sqrt{432}} + o\left(e^x\right), \quad x \to \infty.$$

1.2. Weighted random walks on graphs

Let $\alpha \in \mathcal{E}$ be an edge which originates at $i \in \mathcal{V}$. Denote by $p_{i\alpha} > 0$ the probability that a walker who is passing through vertex i chooses to continue his walk through edge α, and assume that the sum of the probabilities over all edges originating at a given vertex is less than or equal to 1, for all vertices in G. Let $\alpha_1, \ldots, \alpha_k$ be the edges connecting vertex i to vertex j. The graph probability matrix function $N : \mathbb{C} \to M_n(\mathbb{C})$ is defined by

$$N_{ij}(s) = p_{i\alpha_1} e^{-s \cdot l(\alpha_1)} + \cdots + p_{i\alpha_k} e^{-s \cdot l(\alpha_k)}$$

and $N_{ij}(s) = 0$ if i is not connected to j by an edge. Note that the restriction of N to $\mathbb{R}$ is real valued. If the sum of the probabilities over all edges originating at a given vertex is strictly less than 1, there is a positive probability that the walker does not choose any of the edges and instead leaves the graph.

Theorem 2. *Let G be a strongly connected incommensurable graph, and consider a walker on G advancing at constant speed 1. There exist a non-positive constant λ and a matrix $Q \in M_n(\mathbb{R})$ with positive entries such that*

(i) *The probability that a walker leaving $i \in \mathcal{V}$ at time $t = 0$ is exactly at $j \in \mathcal{V}$ at time $t = T$ decays as*

$$Q_{ij} e^{\lambda T} + o\left(e^{\lambda T}\right), \quad T \to \infty$$

for values of T in the countable set of times for which this probability is non-zero.

(ii) *Let $\alpha \in \mathcal{E}$ be an edge in G which originates in vertex $j \in \mathcal{V}$. The probability that a walker who has left some vertex $i \in \mathcal{V}$ at time $t = 0$ is on the edge $\alpha \in \mathcal{E}$ at time $t = T$, where α originates at j and has probability $p_{j\alpha}$, decays as*

$$p_{j\alpha} \frac{1 - e^{-l(\alpha)\lambda}}{\lambda} Q_{ij} e^{\lambda T} + o\left(e^{\lambda T}\right), \quad T \to \infty$$

whenever $\lambda < 0$. In the case $\lambda = 0$, the probability tends to

$$p_{j\alpha} l(\alpha) Q_{ij}, \quad T \to \infty.$$

As in the previous theorem, the constant λ is the maximal real value for which the spectral radius of N is equal to 1, and

$$Q = Q(N(\lambda)) = \frac{\operatorname{adj}(I - N(\lambda))}{-\operatorname{tr}(\operatorname{adj}(I - N(\lambda)) \cdot N'(\lambda))}.$$

As a direct corollary we have

Corollary 1. *In the settings of the previous theorem, denote by $\mathcal{E}(j)$ the set of edges in G with origin at vertex $j \in \mathcal{V}$. The probability that a walker who has left vertex $i \in \mathcal{V}$ at time zero is still on the graph G at time T decays as*

$$\sum_{j \in \mathcal{V}} \sum_{\alpha \in \mathcal{E}(j)} p_{j\alpha} \frac{1 - e^{-l(\alpha)\lambda}}{\lambda} Q_{ij} e^{\lambda T} + o\left(e^{\lambda T}\right), \quad T \to \infty$$

whenever $\lambda < 0$.

Remark 1. It will follow from Remark 4 that in the case $\lambda = 0$ the matrix $N(0)$ is right stochastic and that the probability described in the previous corollary is 1.

The random walk defined above can be generalized by considering a random walk on the edges, and the transition probability $p_{\beta,\alpha}$ from an edge α to an edge β vanishes unless β originates at the vertex where α terminates. Let d be the number of directed edges on the graph. The graph probability matrix function $W : \mathbb{C} \to M_d(\mathbb{C})$ is defined by

$$W_{\beta,\alpha}(s) = p_{\beta,\alpha} e^{-s \cdot l(\alpha)}.$$

The analogues of Theorem 2 and its Corollary 1 in the present case follow directly from the discussion above.

2. Matrices, Perron–Frobenius Theory and Graphs

A real valued matrix $A \in M_n(\mathbb{R})$ is called **positive** if all entries of A are positive and **non-negative** if all entries of A are non-negative. A is called **primitive** if there exists $k \in \mathbb{N}$ for which A^k is positive and **irreducible** if for every pair of indices i, j there exists $k \in \mathbb{N}$ for which $\left(A^k\right)_{ij} > 0$.

2.1. The Perron–Frobenius Theorem

The following results are due to Perron and Frobenius (full statements and proofs can be found in [7, Chap. XIII]).

Theorem. *Let $A \in M_n(\mathbb{R})$ be a **non-negative** and **irreducible** matrix.*

1. *There exists $\mu > 0$ which is a simple eigenvalue of A, and $|\mu_j| \leq \mu$ for any other eigenvalue μ_j. We call μ the **Perron–Frobenius eigenvalue**.*
2. *There exist $v, u \in \mathbb{R}^n$ with positive entries such that $Av = \mu v$ and $u^T A = \mu u^T$. Moreover every right eigenvector with non-negative entries must be a positive multiple of v (similarly for left eigenvectors and u).*

Theorem. *Let $A \in M_n(\mathbb{R})$ be a **primitive** matrix.*

1. *There exists $\mu > 0$ which is a simple eigenvalue of A, and $|\mu_j| < \mu$ for any other eigenvalue μ_j. We call μ the **Perron–Frobenius eigenvalue**.*
2. *There exist $v, u \in \mathbb{R}^n$ with positive entries such that $Av = \mu v$ and $u^T A = \mu u^T$. Moreover every right eigenvector with non-negative entries must be a positive multiple of v (similarly for left eigenvectors and u).*
3. *The following limit holds*

$$\lim_{k\to\infty} \left(\frac{1}{\mu} A\right)^k = \frac{vu^T}{u^T v}.$$

*The limit matrix $P = \frac{vu^T}{u^T v}$ is called the **Perron projection** of A.*

2.2. Perron's projection

Given an irreducible matrix A, there are additional ways to represent its Perron projection P, as shown bellow

Lemma 1. *Let A be an irreducible matrix with Perron–Frobenius eigenvalue μ and a Perron projection P. Then*

$$P = \frac{\operatorname{adj}(\mu I - A)}{\operatorname{tr}(\operatorname{adj}(\mu I - A))}.$$

Proof. Let v and u be eigenvectors as in the Perron–Frobenius theorem. The columns of P are scalar multiples of v, and the rows of P are scalar multiples of u^T, and so the column space of P is spanned by v and the row space by u. Denote by V the subspace of $M_n(\mathbb{R})$ consisting of matrices with these row and column spaces, and notice that $\dim V = 1$. Since μ is an eigenvalue of A we have

$$(\mu I - A) \cdot \operatorname{adj}(\mu I - A) = \det(\mu I - A) I = 0,$$

and so every column of $\operatorname{adj}(\mu I - A)$ is an eigenvector of A corresponding to μ. By the Perron–Frobenius theorem all columns of $\operatorname{adj}(\mu I - A)$ must be scalar multiples of v and so the column space of $\operatorname{adj}(\mu I - A)$ is spanned by v. Similarly, using $\operatorname{adj}(\mu I - A)\cdot(\mu I - A) = 0$ we deduce that the row space of $\operatorname{adj}(\mu I - A)$ is spanned by u, and so $\operatorname{adj}(\mu I - A) \in V$. Since V is one dimensional $\operatorname{adj}(\mu I - A) = \alpha P$ for some $\alpha \in \mathbb{R}$. Next, since $Pv = v$, and $Pw = 0$ for every $w \in (\operatorname{span}\{u\})^{\perp}$, the Perron projection P is similar to the matrix $\operatorname{diag}(1, 0, \ldots, 0)$. Therefore $\operatorname{tr}P = 1$, and so

$$\operatorname{tr}(\operatorname{adj}(\mu I - A)) = \operatorname{tr}(\alpha P) = \alpha \operatorname{tr}P = \alpha,$$

finishing the proof. □

Corollary 2. *Let p_A be the characteristic polynomial of A, then*

$$P = \frac{\operatorname{adj}(\mu I - A)}{\frac{d}{dx} p_A(x)|_{x=\mu}}.$$

Proof. Jacobi's formula for the derivative of the determinant of a matrix is given by

$$\frac{d}{dx}\det B(x) = \operatorname{tr}(\operatorname{adj}(B(x))\, B'(x))$$

and so using this formula, the corollary follows from the previous lemma for $B(x) = xI - A$. □

Remark 2. This result and others concerning the theory of Perron–Frobenius may be found in [19]. Another proof for Corollary 2 can be derived by direct computation using the following identity

$$\operatorname{adj}(\lambda I - A) = A^{n-1} + (\lambda + p_{n-1}) A^{n-2} + \cdots + \left(\lambda^{n-1} + p_{n-1}\lambda^{n-2} + \cdots + p_1\right) I$$

where $p_A(x) = x^n + p_{n-1}x^{n-1} + \cdots + p_0$ and $\lambda \in \mathbb{R}$ (see [7] or [6]). Let μ be the Perron–Frobenius eigenvalue and v a corresponding eigenvector, we compute

$$\begin{aligned} &\operatorname{adj}(\mu I - A)\, v \\ &\quad = \left[\mu^{n-1} + (\mu + p_{n-1})\,\mu^{n-2} + \cdots + \left(\mu^{n-1} + p_{n-1}\mu^{n-2} + \cdots + p_1\right)\right] v \\ &\quad = \left[n\mu^{n-1} + (n-1)\, p_{n-2}\mu^{n-3} + \cdots + p_1\right] v \\ &\quad = p_A'(\mu)\, v. \end{aligned} \tag{2.1}$$

Recall that $\operatorname{adj}(\mu I - A) = \alpha P$ for some $\alpha \in \mathbb{R}$. Since

$$p_A'(\mu)\, v = \operatorname{adj}(\mu I - A)\, v = \alpha P v = \alpha v,$$

it follows that $\alpha = \operatorname{tr}(\operatorname{adj}(\mu I - A)) = p_A'(\mu)$.

Corollary 3. *Let $(\mu, \mu_2, \ldots, \mu_n)$ be the eigenvalues of A, perhaps with repetitions. Then*

$$P = \frac{\prod (A - \mu_i I)}{\prod (\mu - \mu_i)}.$$

Proof. Using the representation of $\operatorname{adj}(\mu I - A)$ as a polynomial of degree $n-1$, it follows from Vieta's polynomial formulas (see, for example, [25]) that

$$\operatorname{adj}(\mu I - A) = (A - \mu_2 I) \cdots (A - \mu_n I).$$

Since $p'_A(\mu) = (\mu - \mu_2) \cdots (\mu - \mu_n)$, this gives the desired result. □

2.3. Comparison between the non-weighted case and the weighted case

When considering path counting questions on a non-weighted graph G, it is often convenient to define its adjacency matrix. This is the square matrix $A \in M_n(\mathbb{R})$ indexed by the vertices of G, where A_{ij} is set as the number of edges from vertex i to vertex j. Note that an adjacency matrix of a strongly connected graph is irreducible, but not necessarily primitive. For primitivity of the adjacency matrix we must also assume that G is aperiodic, which means that the greatest common divisor of the set of lengths of all closed paths is 1.

Recall that the number of paths from vertex i to vertex j consisting of exactly k edges is exactly $\left(A^k\right)_{ij}$. It follows that if the graph is strongly connected and aperiodic, then A is primitive, and by the Perron–Frobenius theorem this number can be approximated by $P_{ij}\mu^k$, where P is the Perron projection of A described above and μ is the Perron–Frobenius eigenvalue.

It is interesting to compare the matrices P and Q, where Q is the matrix defined in the statement of Theorem 1. Due to Jacobi's formula, we can write

$$Q = \frac{\operatorname{adj}(I - M(\lambda))}{-\operatorname{tr}(\operatorname{adj}(I - M(\lambda)) \cdot M'(\lambda))} = \frac{\operatorname{adj}(I - M(\lambda))}{\frac{d}{ds}(\det(I - M(s)))\,|_{s=\lambda}},$$

$$P = \frac{\operatorname{adj}\left(I - \frac{1}{\mu}A\right)}{\operatorname{tr}\left(\operatorname{adj}\left(I - \frac{1}{\mu}A\right)\right)} = \frac{\operatorname{adj}\left(I - \frac{1}{\mu}A\right)}{\frac{d}{dx}\det\left(I - \frac{1}{x}\frac{A}{\mu}\right)|_{x=1}},$$

and the resemblance is clear.

Note that in the case of a non-weighted graph G we assume that G is strongly connected and aperiodic in order to guarantee convergence of $\frac{1}{\mu^k}A^k$ to P, otherwise the corresponding adjacency matrix need not be primitive and the Perron–Frobenius theorem may not be implied. In the case of weighted graphs we change the assumption that G is aperiodic with that of incommensurability.

As an example we look at the following case: Assume all edges in G are of equal length $a > 0$. So $M(s) = e^{-as}A$ where A is the adjacency matrix of the underlying non-weighted graph. Obviously, G is not incommensurable and the assumptions of Theorem 1 do not hold, but still we can calculate Q.

Let μ be the Perron–Frobenius eigenvalue of A, then the matrix $M\left(\frac{\log\mu}{a}\right) = \frac{1}{\mu}A$ has Perron–Frobenius eigenvalue 1, and so $\lambda = \frac{\log\mu}{a}$. Since

$$\begin{aligned}-\mathrm{tr}\left(\mathrm{adj}\left(I - M\left(\lambda\right)\right)\cdot M'\left(\lambda\right)\right) &= -\mathrm{tr}\left(\mathrm{adj}\left(I - \frac{1}{\mu}A\right)\cdot\frac{-a}{\mu}A\right)\\ &= a\,\mathrm{tr}\left(\mathrm{adj}\left(I - \frac{1}{\mu}A\right)\cdot\frac{1}{\mu}A\right)\\ &= a\,\mathrm{tr}\left(\mathrm{adj}\left(I - \frac{1}{\mu}A\right)\right),\end{aligned}$$

we get

$$Q = \frac{\mathrm{adj}\left(I - M\left(\lambda\right)\right)}{-\mathrm{tr}\left(\mathrm{adj}\left(I - M\right)\cdot M'\left(\lambda\right)\right)} = \frac{\mathrm{adj}\left(I - \frac{1}{\mu}A\right)}{a\mathrm{tr}\left(\mathrm{adj}\left(I - \frac{1}{\mu}A\right)\right)} = \frac{1}{a}P,$$

and so if we think of a non-weighted graph as a weighted graph with edges all of length $a = 1$, we get $P = Q$.

3. The Wiener–Ikehara Theorem and the Laplace Transform

3.1. The Wiener–Ikehara Theorem

The proofs of our main results follow from this Tauberian theorem due to Wiener and Ikehara (see [13, Chap. 8.3]).

Theorem. *Let $f(x)$ be a non-negative and monotone function on $[0,\infty)$. Suppose that the Laplace transform of $f(x)$, given by*

$$F(s) := \mathcal{L}\left\{f\left(x\right)\right\}(s) = \int_0^\infty f\left(x\right)e^{-xs}dx,$$

converges for all s with $Re(s) > \lambda$, and that there exists $c \in \mathbb{R}$ for which the function

$$F(s) - \frac{c}{s-\lambda}$$

extends to a continuous function in the closed half-plane $Re(s) \geq \lambda$. Then

$$f\left(x\right) = ce^{\lambda x} + o\left(e^{\lambda x}\right), \quad x \to \infty.$$

3.2. The Laplace Transform of the counting and probability functions

Denote by $\Gamma\left(i,j\right)$ the set of paths originating at vertex $i \in \mathcal{V}$ and terminating at vertex $j \in \mathcal{V}$, and by $p\left(\gamma\right)$ the product of probabilities of the edges which define the path γ.

Let $A_{i,j}(x)$ denote the number of paths originating at vertex i and ending at vertex j of length at most x. Then

$$A_{i,j}(x) = \sum_{\gamma\in\Gamma(i,j)} \chi_{[l(\gamma),\infty)}(x) = \sum_{k=0}^{\infty} \sum_{\substack{\gamma\in\Gamma(i,j)\\ \text{with } k \text{ edges}}} \chi_{[l(\gamma),\infty)}(x)$$

where χ_A is the characteristic function of the set $A \subset \mathbb{R}$. The Laplace transform is

$$\mathcal{L}\{A_{i,j}(x)\}(s) = \sum_{k=0}^{\infty} \sum_{\substack{\gamma\in\Gamma(i,j)\\ \text{with } k \text{ edges}}} \frac{1}{s} e^{-l(\gamma)s} = \frac{1}{s} \left(\sum_{k=0}^{\infty} M^k(s) \right)_{i,j}.$$

Let α be an edge originating at vertex j. Denote by $B_{i,\alpha}(x)$ the number of paths of length exactly x from vertex i to a point on the edge α. Then

$$B_{i,\alpha}(x) = \sum_{\gamma\in\Gamma(i,j)} \chi_{[l(\gamma),l(\gamma)+l(\alpha))}(x) = \sum_{k=0}^{\infty} \sum_{\substack{\gamma\in\Gamma(i,j)\\ with\ k\ edges}} \chi_{[l(\gamma),l(\gamma)+l(\alpha))}(x).$$

The Laplace transform is

$$\mathcal{L}\{B_{i,\alpha}(x)\}(s) = \sum_{k=0}^{\infty} \sum_{\substack{\gamma\in\Gamma(i,j)\\ \text{with } k \text{ edges}}} \frac{1-e^{-l(\alpha)s}}{s} e^{-l(\gamma)s} = \frac{1-e^{-l(\alpha)s}}{s} \left(\sum_{k=0}^{\infty} M^k(s) \right)_{i,j}.$$

Denote by $C_{i,j}(T)$ the probability that a walker leaving i at time zero and moving along the the graph at speed 1, would at time T be exactly at vertex j. Then

$$C_{i,j}(T) = \sum_{\gamma\in\Gamma(i,j)} p(\gamma)\,\delta(T-l(\gamma)) = \sum_{k=0}^{\infty} \sum_{\substack{\gamma\in\Gamma(i,j)\\ \text{with } k \text{ edges}}} p(\gamma)\,\delta(T-l(\gamma))$$

where $\delta(x-a)$ is the delta function centered at $a \in \mathbb{R}$. The Laplace transform is

$$\mathcal{L}\{C_{i,j}(T)\}(s) = \sum_{k=0}^{\infty} \sum_{\substack{\gamma\in\Gamma(i,j)\\ \text{with } k \text{ edges}}} p(\gamma)\, e^{-l(\gamma)s} = \left(\sum_{k=0}^{\infty} N^k(s) \right)_{i,j}.$$

Denote by $D_{i,\alpha}(T)$ the probability that a walker leaving i at time zero and moving along the graph at speed 1, would at time T be on the edge α which originates at vertex j. Then

$$\begin{aligned} D_{i,\alpha}(T) &= \sum_{\gamma\in\Gamma(i,j)} p(\gamma)\, p_{ij} \chi_{[l(\gamma),l(\gamma)+l(\alpha))}(T) \\ &= p_{ij} \sum_{k=0}^{\infty} \sum_{\substack{\gamma\in\Gamma(i,j)\\ \text{with } k \text{ edges}}} p(\gamma)\, \chi_{[l(\gamma),l(\gamma)+l(\alpha))}(T). \end{aligned}$$

The Laplace transform is

$$\mathcal{L}\left\{D_{i,\alpha}\left(T\right)\right\}\left(s\right) = \sum_{k=0}^{\infty} \sum_{\substack{\gamma\in\Gamma(i,j) \\ \text{with } k \text{ edges}}} p_{j\alpha}\frac{1-e^{-l(\alpha)s}}{s}p\left(\gamma\right)e^{-l(\gamma)s}$$

$$= p_{j\alpha}\frac{1-e^{-l(\alpha)s}}{s}\left(\sum_{k=0}^{\infty} N^k\left(s\right)\right)_{i,j}.$$

It will be shown that the sums $\sum_{k=0}^{\infty} M^k\left(s\right)$ and $\sum_{k=0}^{\infty} N^k\left(s\right)$ converge absolutely for suitable values of s, and so we can change the order of summation and integration as implied in the calculations above.

We will show that the constant λ as described in the statement of Theorems 1 and 2 exists, and that these Laplace transforms satisfy the conditions of the Wiener–Ikehara theorem with a simple pole at $s = \lambda$.

4. Proof of main results

Although some of the following results can be found in the literature, we include the full details for the sake of clarity.

Lemma 2. *The matrix elements of powers of $M\left(s\right)$ for $s = \sigma + \mathbf{i}t$ (resp., $N\left(s\right)$) are bounded in absolute value by the corresponding matrix elements of powers of $M\left(\sigma\right)$ (resp., $N\left(\sigma\right)$).*

Proof. Indeed for every $k \in \mathbb{N}$

$$\begin{aligned}\left|\left(M^k\left(s\right)\right)_{ij}\right| &= \left|\sum_{i_1,..,i_{k-1}} M_{i,i_1}\left(s\right)\cdots M_{i_{k-1},j}\left(s\right)\right| \\ &\leq \sum_{i_1,..,i_{k-1}} \left|M_{i,i_1}\left(s\right)\right|\cdots\left|M_{i_{k-1},j}\left(s\right)\right| \\ &\leq \sum_{i_1,..,i_{k-1}} M_{i,i_1}\left(\sigma\right)\cdots M_{i_{k-1},j}\left(\sigma\right) = \left(M^k\left(\sigma\right)\right)_{ij}\end{aligned}$$

and similarly for N, as required. ☐

Remark 3. This lemma is contained in a result due to Wielandt which can be found in [7].

For $\sigma \in \mathbb{R}$ the matrices $M\left(\sigma\right)$ and $N\left(\sigma\right)$ are real, non-negative and irreducible (because the graph G is strongly connected), and so by Perron–Frobenius there exists a dominant real eigenvalue $\mu\left(\sigma\right)$ of multiplicity 1 corresponding to a positive eigenvector $v\left(\sigma\right)$.

Lemma 3. *Let $M\left(\sigma\right)$ be as above. Then there exists $\lambda > 0$ such that $\mu\left(\lambda\right) = 1$ and for every $\sigma > \lambda$ the corresponding dominant eigenvalue satisfies $\mu\left(\sigma\right) < 1$.*

Proof. For all $\sigma \in \mathbb{R}$ there exists $\mu(\sigma)$ which by Perron–Frobenius is a simple eigenvalue of $M(\sigma)$. Let $v(\sigma)$ and $u(\sigma)$ be right and left positive eigenvectors, then since $M(\sigma)$ is differentiable, then by [10, Theorem 6.3.12], $\mu(\sigma)$ is differentiable and the following formula holds

$$\frac{d}{d\sigma}\mu(\sigma) = \frac{u^T(\sigma) M'(\sigma) v(\sigma)}{u^T(\sigma) v(\sigma)}.$$

Since the eigenvectors are positive, and the entry-wise derivative of M is non-positive, we deduce that

$$\frac{d}{d\sigma}\mu(\sigma) < 0 \tag{4.1}$$

so in particular μ is monotone decreasing. Recall that $\mu(0)$ is the largest eigenvalue of the adjacency matrix $M(0)$ of the strongly connected and incommensurable graph G and so $\mu(0) > 1$. Moreover, since all elements of $M(\sigma)$ tend to zero as σ tends to infinity, so does the Perron–Frobenius eigenvalue. Therefore there exists a finite $\lambda > 0$ for which $\mu(\lambda) = 1$ and $\mu(\sigma) < 1$ for all $\sigma > \lambda$. □

Lemma 4. *Let $N(\sigma)$ be as above. Then there exists $\lambda \leq 0$ such that $\mu(\lambda) = 1$ and for every $\sigma > \lambda$ the corresponding dominant eigenvalue satisfies $\mu(\sigma) < 1$.*

Proof. The proof is similar to the discussion about $M(\sigma)$, only here we must show that $\mu(0) \leq 1$ to verify that the value of λ for which $\mu(\lambda) = 1$ is negative. This follows from our assumption that the sum of the probabilities of edges originating at a given vertex is less or equal to 1, and so the sum of the entries of any row in $N(0)$ is bounded by 1, therefore $\mu(0)$ is bounded by 1 (see Wielandt's proof of Perron–Frobenius theorem which appears in [7]). □

Remark 4. Clearly, $\mu(0) = 1$ if and only if the sum of all probabilities for edges originating at vertex i is 1, for all i. In other words $\lambda = 0$ if and only if $N(0)$ is a right stochastic matrix, that is all its rows sum up to 1.

The following lemmas are stated for M, but analogous statements and their proofs apply for N.

Lemma 5. *Let $\lambda \in \mathbb{R}$ be as in Lemma 3. Then $\sum_{k=0}^{\infty} M^k(\sigma)$ converges for all $s = \sigma + \mathbf{i}t$ with $\sigma > \lambda$, and in this case*

$$\sum_{k=0}^{\infty} M^k(s) = (I - M(s))^{-1} = \frac{\operatorname{adj}(I - M(s))}{\det(I - M(s))},$$

and so the Laplace transforms of the counting functions described above are analytic in the half plane $\sigma > \lambda$.

Proof. The lemma follows because for $\sigma > \lambda$, as in Lemma 3, the geometric sum $\sum_{k=0}^{\infty} M^k(\sigma)$ converges, and by Lemma 2 so does $\sum_{k=0}^{\infty} M^k(s)$. □

Plugging the previous statement in the expressions derived in the previous section for the Laplace transforms of the counting functions we study, we conclude the following corollary.

Corollary 4. *Let $A_{i,j}(x)$, $B_{i,\alpha}(x)$, $C_{i,j}(T)$ and $D_{i,\alpha}(T)$ be the counting functions defined in Sect.* 3.2. *The associated Laplace transforms are given by*

$$\mathcal{L}\{A_{i,j}(x)\}(s) = \frac{1}{s}\cdot\frac{(\mathrm{adj}\,(I-M(s)))_{ij}}{\det(I-M(s))},$$
$$\mathcal{L}\{B_{i,\alpha}(x)\}(s) = \frac{1-e^{-l(\alpha)s}}{s}\cdot\frac{(\mathrm{adj}\,(I-M(s)))_{ij}}{\det(I-M(s))},$$
$$\mathcal{L}\{C_{i,j}(T)\}(s) = \frac{(\mathrm{adj}\,(I-N(s)))_{ij}}{\det(I-N(s))},$$
$$\mathcal{L}\{D_{i,\alpha}(T)\}(s) = p_{j\alpha}\frac{1-e^{-l(\alpha)s}}{s}\cdot\frac{(\mathrm{adj}\,(I-N(s)))_{ij}}{\det(I-N(s))},$$

where $\frac{1-e^{\;l(\alpha)s}}{s}$ *is an entire function with value $l(\alpha)$ at $s=0$.*

Lemma 6. *The matrix* $\mathrm{adj}\,(I-M(\lambda))$ *has positive entries.*

Proof. Recall that $\mu(\lambda)=1$, and so by Lemma 1 there exist positive vectors v, u such that

$$\frac{\mathrm{adj}\,(I-M(\lambda))}{\mathrm{tr}\,(\mathrm{adj}\,(I-M(\lambda)))} = \frac{vu^T}{u^Tv}.$$

It follows that all the entries of $\mathrm{adj}\,(I-M(\lambda))$ are non-zero and have the same sign as $\mathrm{tr}\,(\mathrm{adj}\,(I-M(\lambda)))$, which is $\frac{d}{dx}p_{M_G(\lambda_G)}(x)\,|_{x=1}$ by Jacobi's formula. But 1 is a simple root of the characteristic polynomial and is the largest one, and therefore its derivative at $x=1$ is positive. □

Lemma 7. *The Laplace transforms of the graph counting functions $A_{i,j}(x)$ and $B_{i,\alpha}(x)$ have a simple pole at λ.*

Proof. The point $s=\lambda$ is a singular point of the Laplace transforms, because by the previous lemma the numerator $(\mathrm{adj}\,(I-M(\lambda)))_{ij}$ is non-zero while the denominator has a zero at λ. So it is enough to show that the zero of $\det(I-M(s))$ at λ is a simple one. For $\sigma\in\mathbb{R}$, the characteristic polynomial of $M(\sigma)$ is given by

$$p_{M(\sigma)}(x) = \det(xI-M(\sigma)) = (x-\mu(\sigma))(x-\mu_2(\sigma))\cdots(x-\mu_n(\sigma)),$$

where $\mu(\sigma)$ is the Perron–Frobenius eigenvalue of $M(\sigma)$. Therefore $\mu(\lambda)=1$, and $\mu_j(\sigma)\neq 1$ for $j\geq 2$ in a small neighborhood of λ, and

$$\det(I-M(\sigma)) = (1-\mu(\sigma))\cdots(1-\mu_n(\sigma)).$$

It follows from equation (4.1) that the function $(1-\mu(\sigma))$ has a simple zero at λ, and the same holds for the function $\det(I-M(\sigma))$ and therefore also for $\det(I-M(s))$. □

Lemma 8. *For all $t\neq 0$,*

$$\det(I-M(\lambda+\mathbf{i}t))\neq 0,$$

that is, the Laplace transforms have no other poles on the line $Re(s)=\lambda$ than at $s=\lambda$ itself.

Proof. Say that G has the **single-edge property** if for every pair of vertices i, j in G there is at most one edge from vertex i to vertex j. Given a graph G, we define a graph $\widetilde{G}$ by adding a new vertex in the middle of every edge in G. There is a natural one to one map between paths in G and paths in $\widetilde{G}$ which originate and terminate in the original set of vertices, and clearly $\widetilde{G}$ has the single-edge property. Therefore, there is no loss of generality assuming that this property holds for G.

Put $M_{ij} = (M(\lambda))_{ij}$. Since G has the single-edge property, the entries of the matrix $M(\lambda)$ are either $M_{ij} = e^{-\lambda \cdot l(\alpha)}$ if there is an edge $\alpha \in \mathcal{E}$ connecting the vertex i to the vertex j, or $M_{ij} = 0$ if there is no such edge. Let $v = (v_1, ..., v_n)$ be a positive eigenvector of $M(\lambda)$ corresponding to the eigenvalue $\mu(\lambda) = 1$ and define D to be the following invertible matrix

$$D = \operatorname{diag}(v_1, \ldots, v_n), \quad D^{-1} = \operatorname{diag}\left(\frac{1}{v_1}, \ldots, \frac{1}{v_n}\right).$$

The matrix given by $S = D^{-1}MD$ is a non-negative and right stochastic matrix. Indeed, since $S_{ij} = M_{ij}v_j/v_i$, it is clear that $S_{ij} \geq 0$ and that the sum of the elements of the ith row is

$$\sum_{j=1}^{n} S_{ij} = \sum_{j=1}^{n} M_{ij}\frac{v_j}{v_i} = \frac{1}{v_i}\sum_{j=1}^{n} M_{ij}v_j = \frac{v_i}{v_i} = 1.$$

Let $S(s)$ be the matrix with coefficients from S raised to the power of s, that is,

$$(S(s))_{ij} = (S_{ij})^s = (M_{ij})^s \left(\frac{v_j}{v_i}\right)^s.$$

Notice that

$$S(s) = (D^s)^{-1} M(\lambda s) D^s,$$

i.e., $M(\lambda s)$ and $S(s)$ are similar, so in particular they have the same characteristic polynomial $p_{S(s)}(x) = p_{M(\lambda s)}(x)$. Recalling the definition of the characteristic polynomial and plugging $x = 1$, we see that

$$\det(I - M(\lambda s)) = \det(I - S(s)),$$

and so it is enough to show that $\det(I - S(1 + \mathbf{i}t)) \neq 0$ for all $t \neq 0$.

The following argument is due to Parry (see [14]). Assume that

$$\det(I - S(1 + \mathbf{i}t)) = 0 \quad \text{for some } t \neq 0.$$

So there exists a non-zero vector $u = (u_1, \ldots, u_n)$ for which

$$S(1 + \mathbf{i}t)\, u = u,$$

that is, for all i

$$\sum_{j=1}^{n} S_{ij}^{1+\mathbf{i}t} u_j = \sum_{j=1}^{n} S_{ij} S_{ij}^{\mathbf{i}t} u_j = u_i.$$

By the triangle inequality, for all i,

$$|u_i| \leq \sum_{j=1}^{n} \left|S_{ij}^{1+\mathbf{i}t} u_j\right| = \sum_{j=1}^{n} S_{ij} \left|S_{ij}^{\mathbf{i}t}\right| |u_j| = \sum_{j=1}^{n} S_{ij} \, |u_j| \, ,$$

and, together with the equality

$$\sum_{j=1}^{n} S_{ij} = 1,$$

this implies that

$$|u_1| = \cdots = |u_n| \, .$$

Assume $|u_j| = r > 0$ for all j, and notice that this means $S_{ij}^{\mathbf{i}t} u_j$ are points on a circle of radius r. We have therefore that every u_i, which is itself a point on the circle of radius r, is a convex combination (that is, a linear combination with positive coefficients all adding up to 1) of points on that same circle. This is only possible, of course, if $S_{ij}^{\mathbf{i}t} u_j = u_i$ for all j such that $S_{ij} \neq 0$.

Now, for any closed orbit on the graph, let $\alpha_1 = (k_1, k_2), \ldots, \alpha_m = (k_m, k_1)$ denote the corresponding sequence of edges. We get

$$\left(S_{k_1 k_2}^{\mathbf{i}t} u_{k_2}\right) \left(S_{k_2 k_3}^{\mathbf{i}t} u_{k_3}\right) \cdots \left(S_{k_{m-1} k_m}^{\mathbf{i}t} u_{k_m}\right) \left(S_{k_m k_1}^{\mathbf{i}t} u_{k_1}\right) = u_{k_1} u_{k_2} \cdots u_{k_{m-1}} u_{k_m}$$

and so

$$S_{k_1 k_2}^{\mathbf{i}t} \cdots S_{k_m k_1}^{\mathbf{i}t} = \left(S_{k_1 k_2} \cdots S_{k_m k_1}\right)^{\mathbf{i}t} = 1,$$

which gives

$$\left(M_{k_1 k_2} \cdots M_{k_m k_1}\right)^{\mathbf{i}t} = 1.$$

But

$$M_{k_1 k_2} \cdots M_{k_m k_1} = e^{-(l(\alpha_1) + \cdots + l(\alpha_m))}$$

and so there exists some $l \in \mathbb{Z}$ for which

$$t = \frac{2\pi l}{l(\alpha_1) + \cdots + l(\alpha_m)}.$$

This holds for every closed orbit on the graph, yielding a contradiction to our irrationality assumptions on the lengths of the closed orbits on incommensurable graph G. □

Remark 5. When proving the analogous lemma for the case of the matrix N, simply assign the probability 1 to all edges of $\widetilde{G}$ originating at vertices of $\widetilde{G}$ which are not in G.

Remark 6. There is another construction of a graph $\widehat{G}$ associated to G which preserves its structure and has the single-edge property. Let $i \in \mathcal{V}$ be a vertex in G and assume that there are k_i distinct edges which terminate at i and l_i distinct edges which originate at i as shown in Fig. 2.

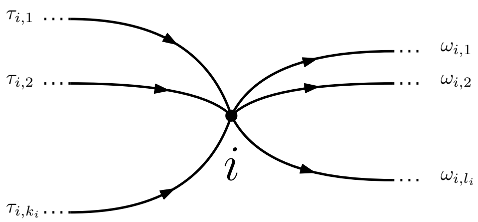

FIGURE 2. Vertex $i \in \mathcal{V}$ and the edges which terminate and originate at i in G

Define $k_i \cdot l_i$ associated vertices in $\widehat{G}$, indexed by

$$\begin{array}{ccc} \tau_{i1} - i - \omega_{i1}, & \dots & \tau_{ik_i} - i - \omega_{i1}, \\ \vdots & & \vdots \\ \tau_{i1} - i - \omega_{il_i}, & \dots & \tau_{ik_i} - i - \omega_{il_i}, \end{array}$$

and repeat this procedure for all vertices in G. Define $\widehat{G}$ to contain a directed edge from $\widehat{v}_1 = \tau_{is} - i - \omega_{it}$ to $\widehat{v}_2 = \tau_{ju} - j - \omega_{jv}$ if and only if $\omega_{it} = \tau_{ju}$. If there is such an edge, and if α is the edge in G for which $\alpha = \omega_{it} = \tau_{ju}$, then the edge between $\widehat{v}_1$ and $\widehat{v}_2$ is labeled by α.

It can be shown that for every path p in G which originates in vertex i and terminates in vertex j, there are exactly $k_i \cdot l_j$ distinct paths in $\widehat{G}$ which are copies of p in the sense of the edges they consist of. It follows that functions counting paths in G which concern vertices i and j differ by a multiplicative constant from the associated functions on $\widehat{G}$, and the same holds for their Laplace transforms. As a result, the position of the poles of the Laplace transforms is not changed.

Lemma 9. *The residue of the function* $\frac{\mathrm{adj}(I-M(s))_{ij}}{\det(I-M(s))}$ *at* $s = \lambda$ *is*

$$Q_{ij} = \frac{(\mathrm{adj}\,(I - M\,(\lambda)))_{ij}}{-\mathrm{tr}\,(\mathrm{adj}\,(I - M\,(\lambda)) \cdot M'\,(\lambda))}.$$

Proof. We have seen that the function has a simple pole at $s = \lambda$, and so the residue at $s = \lambda$ is

$$\frac{(\mathrm{adj}\,(I - M\,(\lambda)))_{ij}}{\frac{d}{ds}\,(\det\,(I - M\,(s)))\,|_{s=\lambda}}.$$

Finally, use Jacobi's formula to obtain

$$\begin{aligned} \frac{d}{ds}\,(\det\,(I - M\,(s))) &= \mathrm{tr}\left(\mathrm{adj}\,(I - M\,(\lambda)) \cdot (I - M\,(s))'\,(\lambda)\right) \\ &= -\mathrm{tr}\,(\mathrm{adj}\,(I - M\,(\lambda)) \cdot M'\,(\lambda))\,. \end{aligned}$$

Combining the above, we get the desired formula for the residue at hand. □

4.1. Proof of Theorems 1 and 2

We show how to conclude the main statements of this paper from the lemmas proven above.

Proof of Theorem 1. Let G be a strongly connected incommensurable graph and let M be the graph matrix function of G. For $\sigma \in \mathbb{R}$ the matrix $M(\sigma)$ is real and due to Perron–Frobenius there exists a dominant real eigenvalue $\mu(\sigma)$ of multiplicity 1. By Lemma 3 there exists $\lambda > 0$ such that $\mu(\lambda) = 1$ and for every $\sigma > \lambda$ the corresponding dominant eigenvalue satisfies $\mu(\sigma) < 1$. By Lemma 2 the series $\sum_{k=0}^{\infty} M^k(s)$ converges for all $s = \sigma + \mathbf{i}t$ with $\sigma > \lambda$ to $\frac{\operatorname{adj}(I-M(s))}{\det(I-M(s))}$ and so by Corollary 4,

$$\mathcal{L}\{A_{i,j}(x)\}(s) = \frac{1}{s} \cdot \frac{(\operatorname{adj}(I - M(s)))_{ij}}{\det(I - M(s))}.$$

By Lemma 7, this $\mathcal{L}\{A_{i,j}(x)\}(s)$ has a simple pole at $s = \lambda$ and by Lemma 8 there are no other poles on the line $\operatorname{Re}(s) = \lambda$. By Lemma 9, the residue of $\mathcal{L}\{A_{i,j}(x)\}(s)$ at $s = \lambda$ is

$$\frac{1}{\lambda} \frac{(\operatorname{adj}(I - M(\lambda)))_{ij}}{-\operatorname{tr}(\operatorname{adj}(I - M(\lambda)) \cdot M'(\lambda))} = \frac{1}{\lambda} Q_{ij}.$$

Therefore applying the Wiener–Ikehara theorem yields statement (i), namely that the number of paths from $i \in \mathcal{V}$ to $j \in \mathcal{V}$ of length at most x grows as

$$\frac{1}{\lambda} Q_{ij} e^{\lambda x} + o\left(e^{\lambda x}\right), \quad x \to \infty.$$

Replacing $A_{i,j}(x)$with $B_{i,j}(x)$ and repeating these steps yields statement (ii), namely that the number of paths of length exactly x from some vertex i to a point on the edge α grows as

$$\frac{1 - e^{-l(\alpha)\lambda}}{\lambda} Q_{ij} e^{\lambda x} + o\left(e^{\lambda x}\right), \quad x \to \infty.$$

□

The proof of Theorem 2 is analogous to the proof of Theorem 1 given above. Lemma 3 is replaced by Lemma 4 and as mentioned above, lemmas analogous to Lemmas 5–9 hold when replacing M with the graph probability matrix function N.

5. Applications

5.1. Summation over regions of Pascal triangle

The well known triangular array of binomial coefficients contains many patterns of numbers and properties of combinatorial interest. It is straightforward to observe that summation of the binomial coefficients in the triangle OBA of sides $OA = \frac{x}{a}$ and $OB = \frac{x}{b}$ (see Fig. 3) is equivalent to counting paths of length at most x in a graph with a single vertex and two loops of lengths a and b.

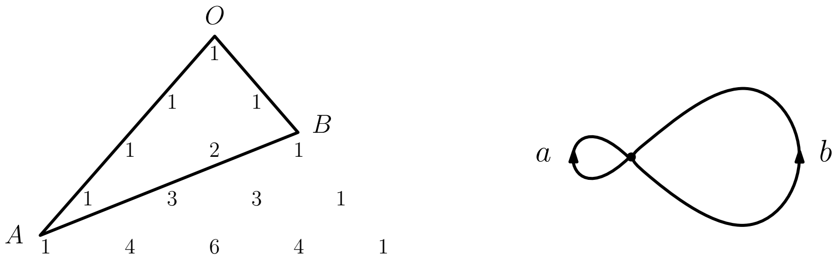

FIGURE 3. A region in Pascal's triangle and the associated graph.

This easily generalizes to Pascal pyramids of higher dimension and weighted graphs with a singe vertex and several loops, and it would be interesting to understand the full correspondence between weighted graphs and regions in Pascal pyramids.

5.2. Multiscale Substitution Schemes

A tile T in $\mathbb{R}^d$ is a Lebegue measurable bounded set with positive measure and boundary of measure zero. Consider a finite set of tiles $\mathcal{F} = \{\mathcal{T}_1, \ldots, \mathcal{T}_n\}$ in $\mathbb{R}^d$ which we call prototiles, and assume for simplicity $\operatorname{vol} \mathcal{T}_i = 1$. A tile T is said to be of type i if it maps to $\mathcal{T}_i$ by a similarity map. A multiscale substitution scheme on $\mathcal{F}$ is a set of substitution rules on elements of $\mathcal{F}$ prescribing a tiling of each prototile by finitely many rescaled copies of tiles of types appearing in $\mathcal{F}$.

A multiscale substitution scheme can be modeled using a directed weighted graph G with a vertex set indexed by elements of $\mathcal{F}$ and an edge set defined by the substitution rule: if the tiling of $\mathcal{T}_i$ includes a tile of type j, that is a copy of $\alpha\mathcal{T}_j$ with $0 < \alpha < 1$, then G admits a directed edge of length $a = -\log \alpha$ connecting vertex i to j. A multiscale substitution scheme is called irreducible if G is strongly connected, and incommensurable if G is incommensurable. An example of an incommensurable multiscale substitution scheme on a single prototile with scales $\alpha_1 = \frac{1}{3}$ and $\alpha_2 = \frac{2}{3}$ is shown in Fig. 4.

Observe that if G is a graph associated with a d dimensional multiscale substitution scheme, then $\lambda = d$ and the Perron–Frobenius eigenvector of $M(d)$ corresponding to $\mu = 1$ can be chosen to be $v = (1, \ldots, 1)$. These properties enable us to address questions concerning the geometrical objects described bellow.

Kakutani Splitting Procedure. Consider the unit interval $I = [0, 1]$ and some $\alpha \in (0, 1)$. Kakutani introduced the following splitting procedure which generates a sequence of partitions of I which is known as the α-Kakutani's sequence of partitions (see [11]). Begin with $\pi_0 = I$ the trivial partition of I, and define π_1 to be the partition of I one gets after splitting I into two intervals of lengths α and $1 - \alpha$. Assume that the partition π_n is defined, then π_{n+1} is the partition of I one

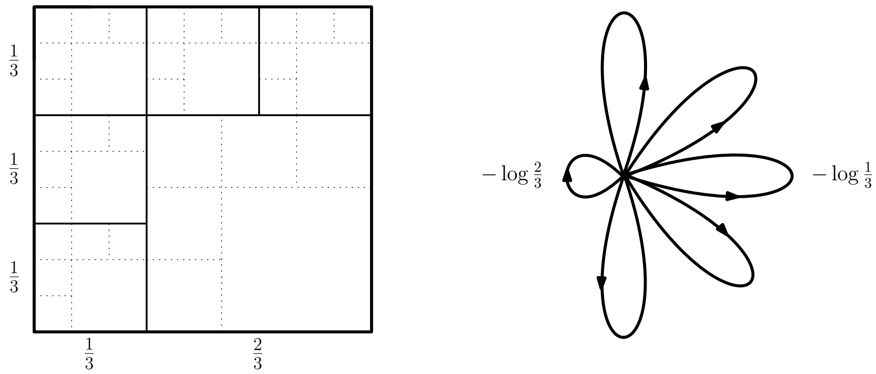

FIGURE 4. A multiscale substitution scheme and the associated graph.

gets from π_n after splitting the interval of maximal length in π_n into two parts, proportional to α and $1 - \alpha$.

For example, the first few α-Kakutani partitions of the unit interval with $\alpha = \frac{1}{3}$ are shown in Fig. 5, together with the associated graph. The dashed lines represent intervals of maximal length in each partition.

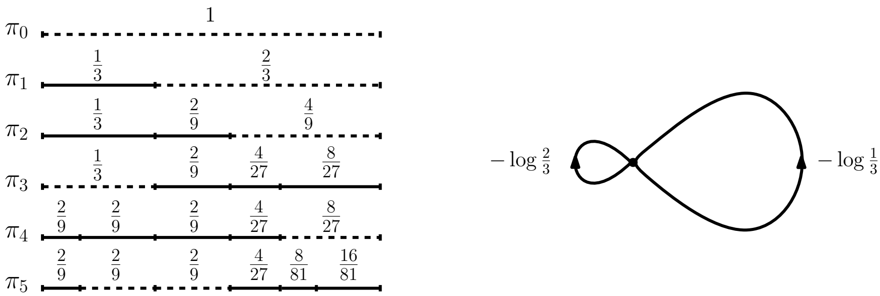

FIGURE 5. The $\frac{1}{3}$-Kakutani sequence of partitions and the associated graph.

We say that a sequence π_n of partitions of I is uniformly distributed if for any continuous function f on I we have

$$\lim_{n\to\infty} \frac{1}{k(n)} \sum_{i=1}^{k(n)} f\left(t_i^{(n)}\right) = \int_I f(t)\, dt$$

where $k(n)$ is the number of intervals in the partition π_n, and $t_i^{(n)}$ is the right endpoint of the ith interval in the partition π_n. The following result is due to Kakutani.

Theorem. *For any $\alpha \in (0,1)$, the α-Kakutani sequence of partitions of I is uniformly distributed.*

Kakutani's splitting procedure is generalized in various ways, see, for example, [5, 26]. An additional generalization comes from multiscale substitution schemes, where we begin with an initial tile $\mathcal{T}_1$, and define a sequence of partitions of $\mathcal{T}_1$ using the substitution rule applied at each stage to tiles of maximal volume. In fact, the example given above of Kakutani's original procedure, can be considered as generated by a multiscale substitution scheme in $\mathbb{R}^1$ with $\mathcal{F} = \{I\}$ the unit interval and $\alpha_1 = \frac{1}{3}$ and $\alpha_2 = \frac{2}{3}$. Theorem 1 is used in [21] to show that such sequences of partitions are uniformly distributed.

Multiscale Substitution Tilings of Euclidean Spaces. A multiscale substitution scheme in $\mathbb{R}^d$ can be used to generate a tiling of the entire space. We define a sequence of tilings of finite regions of $\mathbb{R}^d$ which depends on a continuous time parameter t in the following way: At $t = 0$ apply the substitution rule on an initial tile $\mathcal{T}_1$, and inflate the resulting patch of tiles at a constant speed. Any tile which reaches volume 1 is then substituted as dictated by the multiscale substitution rule, and so on. An appropriate compact topology defined on closed subsets of the space allows us to take limits of sequences of these partial tilings, and these limits define tilings of $\mathbb{R}^d$. The generalization of the pinwheel tiling which is presented in [17] can be regarded as a multiscale substitution tiling.

Although there is no uniqueness in the construction of tilings using multiscale substitutions, all tilings defined this way share various properties which can be analyzed employing the multiscale substitution scheme itself and the underlying weighted graph. For example, tilings which are associated with incommensurable multiscale substitution schemes are of infinite local complexity, unlike classical substitution tilings or tilings defined using cut-and-project constructions (for more on tilings and mathematical models of quasicrystals see [2]). Our Theorem 1 may be used to study various statistics of these tilings, see [22] for more details, and [23] and [24] for relevant results concerning classical substitution tilings.

5.3. Physics Applications

The propagation of radiation pulses through networks of wave-guides requires for its study the full theory of wave dynamics, where interference effects play an important role (see [18] and references therein). However, under certain conditions the interference effects can be neglected, which opens the possibility to study this system within a classical dynamics setting: The network is modeled by a metric, directed graph G, where for any directed edge α connecting vertex u to vertex v, there exists a "reverse" edge $\widehat{\alpha}$ from v to u of the same length. The vertices correspond to the junctions in the network where wave-guides are connected. In the classical model, one considers a point mass moving at a unit speed along a directed edge α, towards the vertex v. Reaching v, the point mass is scattered into any of the edges α' which emanate from v where it continues to move with unit speed. The probabilities to make the transitions from α to α' are prescribed by the properties of the connectors in the wave-guide network.

The network is connected to the outside world through leads which are coupled to a subset of vertices $\mathcal{H}$. One of the vertices $s \in \mathcal{H}$ is connected to a radiation source which sends short pulses to the network at specified times. Another vertex $t \in \mathcal{H}$ is connected to a lead which ends with a detector where the time of arrival is measured. The radiation which is scattered to the leads escapes from the network. In the classical model, a particle is injected to the vertex s at a given time, and once it scattered from t to the lead, its arrival time is measured. Repeating the process one can obtain the probability distribution of the transition times. This model can be analyzed within the formalism provided by Theorem 2.

The complete wave theory and the derivation of the corresponding classical model are provided in [18]. This paper also includes an analysis of a simple network (similar to the one shown here in Fig. 3, with the lead connected at the single vertex) and the transition time distributions computed both in the wave and the classical descriptions are compared.

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Diagonalization of indefinite saddle point forms

Luka Grubišić, Vadim Kostrykin, Konstantin A. Makarov, Stephan Schmitz and Krešimir Veselić

To the memory of Boris Sergeevich Pavlov

Abstract. We obtain sufficient conditions that ensure block diagonalization (by a direct rotation) of sign-indefinite symmetric sesquilinear forms as well as the associated operators that are semi-bounded neither from below nor from above. In the semi-bounded case, we refine the obtained results and, as an example, revisit the block Stokes operator from fluid dynamics.

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1. Introduction

Diagonalizing a quadratic form, which is a classic problem of linear algebra and operator theory, is closely related to the search for invariant subspaces for the (bounded) operator associated with the form. In the Hilbert space setting, a particular case where an invariant subspace can be represented as the graph of a bounded operator acting from a given subspace of the Hilbert space to its orthogonal complement, is of special interest. This situation is quite common while studying block operator matrices, where an orthogonal decomposition of the Hilbert space is available by default. In particular, solving the corresponding invariant graph-subspace problem for bounded self-adjoint block operator matrices automatically yields a block diagonalization of the matrix by a unitary transformation. It is important to note that solving the problem is completely nontrivial even in the bounded case: a self-adjoint operator matrix may have no invariant graph subspace (with respect to

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a given orthogonal decomposition) and, therefore, may not be block diagonalized in this sense, see, e.g., [23, Lemma 4.2].

To describe the block diagonalization procedure in the self-adjoint bounded case in more detail, assume that the Hilbert space $\mathcal{H}$ splits into a direct sum of its subspaces, $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$, and suppose that B is a 2×2 self-adjoint block operator matrix with respect to this decomposition. In the framework of off-diagonal perturbation theory, we also assume that $B = A + V$, with A and V the diagonal and off-diagonal parts of B, respectively.

We briefly recall that the search for an invariant subspace of B that can be represented as the graph of a bounded (angular) operator X acting from $\mathcal{H}_+$ to $\mathcal{H}_-$ is known to be equivalent to finding the skew-self-adjoint "roots"

$$Y := \begin{pmatrix} 0 & -X^* \\ X & 0 \end{pmatrix}$$

of the (algebraic) Riccati equation (see, e.g., [3, 30])

$$AY - YA - YVY + V = 0.$$

Given such a solution Y, one observes that the Riccati equation can be rewritten as the following operator equalities

$$(A+V)(I_{\mathcal{H}}+Y) = (I_{\mathcal{H}}+Y)(A+VY) \quad \text{and} \quad (I_{\mathcal{H}}-Y)(A+V) = (A-YV)(I_{\mathcal{H}}-Y),$$

with $A + VY = (A - YV)^*$ block diagonal operators.

In turn, those operator equalities ensure a block diagonalization of B by the similarity transformation $I \pm Y$, and, as the next step, by the direct rotation U from the subspace $\mathcal{H}_+$ to the invariant graph subspace $\mathcal{G}_+ = \mathrm{Graph}(\mathcal{H}_+, X) := \{x + Xx \mid x \in \mathcal{H}_+\}$ (see [7, 8] for the concept of a direct rotation). Apparently, the direct rotation is given by the unitary operator from the polar decomposition

$$(I + Y) = U|I + Y|.$$

Solving the Riccati equation, the main step of the diagonalization procedure described above, attracted a lot of attention from several groups of researchers.

Different ideas and methods have been used to solve the Riccati equation under various assumptions on the (unbounded) operator B. For an extensive list of references we refer to [3] and [40] (for matrix polynomial and Riccati equations in finite dimension see [9, 13, 14, 15, 16, 28, 34]). For more recent results, in particular on Dirac operators with Coulomb potential, dichtonomous Hamiltonians, and bisectorial operators, we refer to [6, 41, 43, 44].

The most comprehensive results regarding the solvability of the Riccati equation can be obtained under the hypothesis that the spectra of the diagonal part of the operator B restricted to its reducing subspaces $\mathcal{H}_\pm$ are subordinated. For instance, in the presence of a gap separating the spectrum, the Davis-Kahan $\tan 2\Theta$-Theorem [8] can be used to ensure the existence of contractive solutions to the corresponding Riccati equation. In this case, efficient norm bounds for the angular operator can be obtained. The case where there is no spectral gap but the spectra of the diagonal entries have only one-point intersection λ has also been treated, see, e.g., [2, 24], [37, Theorem 2.13], [40, Proposition 2.7.13]. Also, see the recent work [30], where, in particular, the decisive role of establishing the kernel splitting property

$$\mathrm{Ker}(B-\lambda) = (\mathrm{Ker}(B-\lambda) \cap \mathcal{H}_+) \oplus (\mathrm{Ker}(B-\lambda) \cap \mathcal{H}_-)$$

in the diagonalization process is discussed, cf. [40, Sect. 2.7].

In the present paper, we extend the diagonalization scheme to the case of indefinite saddle point forms. Recall that a symmetric saddle point form $\mathfrak{b}$ with respect to the decomposition $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$ is a form sum $\mathfrak{b} = \mathfrak{a} + \mathfrak{v}$, where the diagonal part of the form $\mathfrak{a}$ splits into the difference of two non-negative closed forms in the spaces $\mathcal{H}_+$ and $\mathcal{H}_-$, respectively, and the off-diagonal part $\mathfrak{v}$ is a symmetric form-bounded perturbation of $\mathfrak{a}$.

First, we treat the case where the domain of the form $\mathrm{Dom}[\mathfrak{b}]$ and the form domain $\mathrm{Dom}(|B|^{1/2})$ of the associated operator B defined via the First Representation Theorem for saddle point forms coincide. Putting it differently, we assume that the corresponding Kato square-root problem has an affirmative answer. In this case, we show that on the one hand the semi-definite subspaces

$$\mathcal{L}_\pm = \mathrm{Ran}\,(\mathsf{E}_B(\mathbb{R}_\pm \setminus \{0\})) \oplus \left(\mathrm{Ker}(B) \cap \mathcal{H}_\pm\right) \tag{1.1}$$

reduce both the operator B and the form $\mathfrak{b}$. On the other hand, the semi-positive subspace $\mathcal{L}_+$ is a graph subspace with respect to the decomposition $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$, see Theorem 3.3. Under some additional regularity assumptions, we block diagonalize both the form and the associated operator by the direct rotation from the subspace $\mathcal{H}_+$ to the subspace $\mathcal{L}_+$.

More generally, we introduce the concept of a block form Riccati equation associated with a given saddle point form and relate its solvability to the existence of graph subspaces that reduce the form. Based on these considerations, we block diagonalize the form by a unitary transformation, provided that some regularity requirements are met as well, see Theorem 6.5.

As an application, we revisit the spectral theory for the Dirichlet Stokes block operator (that describes stationary motion of a viscous fluid in a bounded domain $\Omega \subset \mathbb{R}^d$) (see [20], cf. [10]).

$$\begin{pmatrix} -\nu\boldsymbol{\Delta} & v_*\,\mathrm{grad} \\ -v_*\mathrm{div} & 0 \end{pmatrix}$$

in the direct sum of Hilbert spaces $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_- = L^2(\Omega)^d \oplus L^2(\Omega)$.

The paper is organized as follows:

In Sect. 2, we introduce the class of saddle point forms and recall the corresponding Representation Theorems for the associated operators.

In Sect.3, we discuss reducing subspaces for saddle point forms that are the graph of a bounded operator.

In Sect. 4, we recall the concept of a direct rotation and define the class of regular graph decompositions.

In Sect. 5, we block diagonalize the associated operator by a unitary transformation provided that the domain stability condition holds and that the graph decomposition $\mathcal{H} = \mathcal{L}_+ \oplus \mathcal{L}_-$ into the sum of semi-definite subspaces $\mathcal{L}_\pm$ given by (1.1) is regular, see Theorem 5.1.

In Sect. 6, we introduce the concept of a block form Riccati equation and provide sufficient conditions for the block diagonalizability of a saddle point form by a unitary transformation, see Theorem 6.5.

In Sect. 7, we discuss semi-bounded saddle point forms and illustrate our approach on an example from fluid dynamics.

We adopt the following notation. In the Hilbert space $\mathcal{H}$ we use the scalar product $\langle \cdot , \cdot \rangle$ semi-linear the first and linear in the second component. Various auxiliary quadratic forms will be denoted by $\mathfrak{t}$. We write $\mathfrak{t}[x]$ instead of $\mathfrak{t}[x,x]$. $I_\mathfrak{K}$ denotes the identity operator on a Hilbert space $\mathfrak{K}$, where we frequently omit the subscript. If $\mathfrak{t}$ is a quadratic form and S is a bounded operator we define the sum $\mathfrak{t}+S$ as the form sum $\mathfrak{t}+\langle \cdot, S\cdot\rangle$ on the natural domain $\mathrm{Dom}[\mathfrak{t}]$. For operators S and Borel sets M the corresponding spectral projection is denoted by $\mathsf{E}_S(M)$. Given an orthogonal decomposition $\mathfrak{K}_0 \oplus \mathfrak{K}_1$ of the Hilbert space $\mathfrak{K}$ and dense subsets $\mathcal{K}_i \subseteq \mathfrak{K}_i$, $i = 0, 1$, by $\mathcal{K}_0 \oplus \mathcal{K}_1$ we denote a subset of $\mathfrak{K}$ formed by the vectors $\begin{pmatrix} x_0 \\ x_1 \end{pmatrix}$ with $x_i \in \mathcal{K}_i$, $i = 0, 1$. For a self-adjoint operator T we introduce the (Sobolev) space $\mathcal{H}^1_T$ as the set $\mathrm{Dom}(|T|^{1/2})$ equipped with the graph norm.

2. Saddle point forms

To introduce the concept of a saddle point form in a Hilbert space $\mathcal{H}$, we pick up a self-adjoint involution J given by the operator matrix [18],

$$J = \begin{pmatrix} I_{\mathcal{H}_+} & 0 \\ 0 & -I_{\mathcal{H}_-} \end{pmatrix}_{\mathcal{H}_+ \oplus \mathcal{H}_-} \tag{2.1}$$

with respect to a given decomposition of the Hilbert space $\mathcal{H}$ into the orthogonal sum of its closed subspaces

$$\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-. \tag{2.2}$$

A sesquilinear form $\mathfrak{a}$ is called diagonal (with respect to the decomposition (2.2) if the domain $\mathrm{Dom}[\mathfrak{a}]$ is J-invariant and the form $\mathfrak{a}$ "commutes" with the involution J,

$$\mathfrak{a}[x, Jy] = \mathfrak{a}[Jx, y] \quad \text{for} \quad x, y \in \mathrm{Dom}[\mathfrak{a}],$$

and the form

$$\mathfrak{a}_J[x, y] = \mathfrak{a}[x, Jy] \quad \text{on} \quad \mathrm{Dom}[\mathfrak{a}_J] = \mathrm{Dom}[\mathfrak{a}] \tag{2.3}$$

is a closed non-negative form. In particular, the form $\mathfrak{a}$ splits into the difference of closed non-negative forms

$$\mathfrak{a} = \mathfrak{a}_+ \oplus (-\mathfrak{a}_-) \tag{2.4}$$

with respect to the decomposition $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$.

Correspondingly, a sesquilinear form $\mathfrak{v}$ is called off-diagonal if the "anti-commutation relation"

$$\mathfrak{v}[x, Jy] = -\mathfrak{v}[Jx, y] \quad \text{for} \quad x, y \in \mathrm{Dom}[\mathfrak{v}]$$

holds.

We say that a form $\mathfrak{b}$ is a saddle point form with respect to the decomposition (2.2) if it admits the representation

$$\mathfrak{b}[x, y] = \mathfrak{a}[x, y] + \mathfrak{v}[x, y], \quad x, y \in \mathrm{Dom}[\mathfrak{b}] = \mathrm{Dom}[\mathfrak{a}],$$

where $\mathfrak{a}$ is a diagonal form, $\mathfrak{v}$ is a symmetric off-diagonal form and relatively bounded with respect to $\mathfrak{a}_J$,

$$|\mathfrak{v}[x]| \leq \beta(\mathfrak{a}_J[x] + \|x\|^2), \quad x \in \mathrm{Dom}[\mathfrak{v}],$$

for some $\beta \geq 0$. In this case, let $\mathcal{H}_A^1$ denote the set $\mathrm{Dom}[\mathfrak{b}]$ with the graph norm of $|A|^{1/2}$, where

$$A = \begin{pmatrix} A_+ & 0 \\ 0 & -A_- \end{pmatrix} \tag{2.5}$$

is a diagonal operator with respect to the decomposition $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$ and $A_\pm$ are the non-negative self-adjoint operators associated with the closed forms $\mathfrak{a}_\pm$ given by (2.4).

We start by recalling the First and Second Representation Theorem adapted here to the case of saddle point forms (see [37, Theorem 2.7], [18], [19], see also [32]).

Theorem 2.1 (The First Representation Theorem). *Let $\mathfrak{b}$ be a saddle point form with respect to the decomposition $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$.*

Then there exists a unique self-adjoint operator B such that

$$\mathrm{Dom}(B) \subseteq \mathrm{Dom}[\mathfrak{b}]$$

and

$$\mathfrak{b}[x, y] = \langle x, By \rangle \quad \textit{for all} \quad x \in \mathrm{Dom}[\mathfrak{b}] \quad \textit{and} \quad y \in \mathrm{Dom}(B).$$

We say that the operator B associated with the saddle point form $\mathfrak{b}$ via Theorem 2.1 satisfies the *domain stability condition* if the Kato square root problem has an affirmative answer. That is,

$$\mathrm{Dom}[\mathfrak{b}] = \mathrm{Dom}(|B|^{1/2}). \tag{2.6}$$

We note that the domain stability condition may fail to hold for form-bounded but not necessarily off-diagonal perturbations of a diagonal form, see [18, Example 2.11] and [12] for counterexamples.

The corresponding Second Representation Theorem can be stated as follows.

Theorem 2.2 (The Second Representation Theorem). *Let $\mathfrak{b}$ be a saddle point form with respect to the decomposition $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$ and B the associated operator.*

If the domain stability condition (2.6) *holds, then the operator B represents this form in the sense that*

$$\mathfrak{b}[x,y] = \langle |B|^{1/2}x, \operatorname{sign}(B)|B|^{1/2}y\rangle \quad \text{for all } x,y \in \operatorname{Dom}[\mathfrak{b}] = \operatorname{Dom}(|B|^{1/2}).$$

Remark 2.3. Let $\mathfrak{a}$ be a diagonal form and $A = JA_J$, where A_J is a self-adjoint operator associated with the closed non-negative form $\mathfrak{a}_J$ in (2.3). Clearly, the operator A is associated with the form $\mathfrak{a}$ and the form $\mathfrak{a}$ is represented by A as well. Notice that $\mathfrak{a}_J$ is associated in the standard sense with the self-adjoint operator $|A|$.

Next, we present an example of a saddle point form "generated" by an operator.

Example 2.4. Given the decomposition (2.2), suppose that $A_\pm \geq 0$ are self-adjoint operators in $\mathcal{H}_\pm$. Also suppose that

$$W\colon \operatorname{Dom}(W) \subseteq \mathcal{H}_+ \to \mathcal{H}_-$$

is a densely defined closable linear operator such that

$$\operatorname{Dom}(A_+^{1/2}) \subseteq \operatorname{Dom}(W). \tag{2.7}$$

Let $\mathfrak{a}$ be the diagonal saddle point form associated with the diagonal operator

$$A = \begin{pmatrix} A_+ & 0 \\ 0 & -A_- \end{pmatrix}.$$

On

$$\operatorname{Dom}[\mathfrak{b}] = \operatorname{Dom}[\mathfrak{a}] = \operatorname{Dom}(|A|^{1/2})$$

consider the form sum

$$\mathfrak{b} = \mathfrak{a} + \mathfrak{v}, \tag{2.8}$$

where the off-diagonal symmetric perturbation is given by

$$\mathfrak{v}[x,y] = \langle Wx_+, y_-\rangle + \langle x_-, Wy_+\rangle,$$

$$x = x_+ \oplus x_-, \quad y = y_+ \oplus y_-, \quad x_\pm, y_\pm \in \operatorname{Dom}(|A_\pm|^{1/2}) \subseteq \mathcal{H}_\pm.$$

Lemma 2.5. *The form $\mathfrak{b}$ defined by* (2.8) *in Example* 2.4 *is a saddle point form. Moreover, the off-diagonal part $\mathfrak{v}$ of the form $\mathfrak{b}$ is infinitesimally form-bounded with respect to the non-negative closed form $\mathfrak{a}_J$ given by*

$$\mathfrak{a}_J[x,y] = \langle |A|^{1/2}x, |A|^{1/2}y\rangle$$

on $\operatorname{Dom}[\mathfrak{a}_J] = \operatorname{Dom}(|A|^{1/2})$.

Proof. From (2.7) it follows that the operator W is $A_+^{1/2}$-bounded (see [21, Remark IV.1.5]) and therefore

$$\|Wx_+\| \le a\|x_+\| + b\|A_+^{1/2}x_+\|, \quad x_+ \in \mathrm{Dom}(A_+^{1/2}),$$

for some constants a and b. This shows the off-diagonal part $\mathfrak{v}$ of the form $\mathfrak{b}$ is relatively bounded with respect to the diagonal form $\mathfrak{a}_J$ and hence $\mathfrak{b}$ is a saddle point form.

The last assertion follows from the series of inequalities

$$\begin{aligned}|\mathfrak{v}[x]| &\le 2|\langle Wx_+, x_-\rangle| \le 2\|Wx_+\|\cdot\|x_-\| \le 2\big(a\|x_+\| + b\|A_+^{1/2}x_+\|\big)\|x_-\| \\ &= 2a\|x_+\|\cdot\|x_-\| + 2b\sqrt{\mathfrak{a}_+[x_+]}\|x_-\| \\ &\le (a^2+1)\|x\|^2 + \varepsilon b^2\mathfrak{a}_+[x_+] + \frac{\|x\|^2}{\varepsilon}, \\ &\qquad x = x_+ \oplus x_-,\ x_\pm \in \mathrm{Dom}[\mathfrak{a}] \cap \mathcal{H}_\pm\end{aligned}$$

valid for all $\varepsilon > 0$. □

Remark 2.6. The operator B associated with the saddle point form $\mathfrak{b}$ from Example 2.4 can be considered a self-adjoint realization of the "ill-defined" Hermitian operator matrix

$$\dot{B} = \begin{pmatrix} A_+ & W^* \\ W & -A_- \end{pmatrix}. \tag{2.9}$$

Note that in this case we do not impose any condition on $\mathrm{Dom}(A_-)\cap\mathrm{Dom}(W^*)$, so that the "initial" operator $\dot{B}$ is not necessarily densely defined on its natural domain $\mathrm{Dom}(\dot{B}) = \mathrm{Dom}(A_+)\oplus(\mathrm{Dom}(A_-)\cap\mathrm{Dom}(W^*))$. In particular, we neither require that $\mathrm{Dom}(A_-)\supseteq\mathrm{Dom}(W^*)$, cf. [4], nor that $\dot{B}$ is essentially self-adjoint, cf. [40, Theorem 2.8.1].

We close this section by the observation that semi-bounded saddle point forms are automatically closed is the standard sense.

Recall that a linear set $\mathcal{D}\subseteq\mathcal{H}$ is called a core for the semi-bounded from below form $\mathfrak{b}\ge cI_{\mathcal{H}}$ if $\mathcal{D}\subseteq\mathrm{Dom}[\mathfrak{b}]$ is dense in $\mathrm{Dom}[\mathfrak{b}]$ with respect to the norm $||f||_{\mathfrak{b}} = \sqrt{\mathfrak{b}[f] + (1-c)||f||^2}$, see, e.g., [35, Sect. VIII.6].

Lemma 2.7. *Suppose that* $\mathfrak{b}$ *is a semi-bounded saddle point form with respect to the decomposition* $\mathcal{H} = \mathcal{H}_+\oplus\mathcal{H}_-$*. Then* $\mathfrak{b}$ *is closed in the standard sense. In particular, the domain stability condition* (2.6) *automatically holds.*

Moreover, if $\mathcal{D}$ *is a core for the diagonal part* $\mathfrak{a}$ *of the form* $\mathfrak{b}$*, then* $\mathcal{D}$ *is also a core for* $\mathfrak{b}$*.*

Proof. Assume for definiteness that $\mathfrak{b}$ is semibounded from below. Let $\mathfrak{a}$ and $\mathfrak{v}$ be the diagonal and off-diagonal parts of the form $\mathfrak{b}$, respectively.

Since the off-diagonal part $\mathfrak{v}$ is relatively bounded with respect to $\mathfrak{a}_J$, that is,

$$|\mathfrak{v}[x]| \le \beta(\mathfrak{a}_+ + \mathfrak{a}_- + I)[x] = \beta\langle(|A|+I)^{1/2}x, (|A|+I)^{1/2}x\rangle, \quad x\in\mathrm{Dom}[\mathfrak{a}],$$

for some $\beta < \infty$, applying [21, Lemma VI.3.1] shows that $\mathfrak{v}$ admits the representation

$$\mathfrak{v}[x,y] = \langle (|A|+I)^{1/2}x, R(|A|+I)^{1/2}y\rangle, \quad x,y \in \mathrm{Dom}[\mathfrak{a}],$$

with a bounded operator R.

Since $\mathfrak{v}$ is off-diagonal, the operator R is off-diagonal as well, so that

$$JR = -RJ.$$

Introducing the form

$$\widetilde{\mathfrak{b}}[x,y] = \mathfrak{b}[x,y] + \langle x, Jy\rangle, \quad x,y \in \mathrm{Dom}[\mathfrak{a}],$$

one observes that

$$\widetilde{\mathfrak{b}}[x,y] = \langle (|A|+I)^{1/2}x, (J+R)(|A|+I)^{1/2}y\rangle, \quad x,y \in \mathrm{Dom}[\mathfrak{a}].$$

Here we used that

$$\mathfrak{a}[x,y] + \langle x, Jy\rangle = \langle |A|^{1/2}x, J|A|^{1/2}y\rangle + \langle x, Jy\rangle = \langle (|A|+I)^{1/2}x, J(|A|+I)^{1/2}y\rangle$$

for $x,y \in \mathrm{Dom}[\mathfrak{a}]$.

Since the spectrum of J consists of no more than two points ± 1 and the operator R is off-diagonal, the interval $(-1,1)$ belongs to the resolvent set of the bounded operator $J+R$. In particular, $J+R$ has a bounded inverse, see [24, Remark 2.8]. Since $|A|+I$ is strictly positive, applying the First Representation Theorem [18, Theorem 2.3] shows that the self-adjoint operator $\widetilde{B} = (|A|+I)^{1/2}(J+R)(|A|+I)^{1/2}$ is associated with the semi-bounded form $\widetilde{\mathfrak{b}}$ and is semi-bounded as well. Taking into account the one-to-one correspondence between closed semi-bounded forms and semi-bounded self-adjoint operators proves that the form $\widetilde{\mathfrak{b}}$ is closed, so is $\mathfrak{b}$ as a bounded perturbation of a closed form.

To show that any core for the diagonal part $\mathfrak{a}$ is also a core for $\mathfrak{b}$, we remark first that since $\mathfrak{b}$ is semi-bounded from below, the diagonal part $\mathfrak{a}$ of the form $\mathfrak{b}$ is semi-bounded from below as well. Indeed, otherwise, the form $\mathfrak{a}_-$ is not bounded and therefore there is a sequence $x_n \in \mathrm{Dom}[\mathfrak{a}_-]$, $\|x_n\| = 1$, such that $\mathfrak{a}_-[x_n] \to \infty$. In this case,

$$\mathfrak{b}[0 \oplus x_n] = -\mathfrak{a}_-[x_n] \to -\infty,$$

which contradicts the assumption that $\mathfrak{b}$ is a semi-bounded from below form.

Now, since $\mathfrak{b}$ is closed, by [21, Theorem VI.2.23], the domain stability condition (2.6) holds. This means that the spaces $\mathcal{H}_A^1$ and $\mathcal{H}_B^1$ associated with the operators A and B coincide. Hence $\mathcal{D}$ is dense in $\mathcal{H}_A^1$ if and only if it is dense in $\mathcal{H}_B^1$ (w.r.t. the natural topology on the form domain). In other words, $\mathcal{D}$ is a core for the form $\mathfrak{b}$ whenever it is a core for the form $\mathfrak{a}$. $\square$

3. Reducing subspaces

Recall that a closed subspace $\mathfrak{K}$ reduces a self-adjoint operator T if

$$QT \subseteq TQ,$$

where Q is the orthogonal projection in $\mathcal{H}$ onto $\mathfrak{K}$ (see [21, Sect. V.3.9]).

This notion of a reducing subspace $\mathfrak{K}$ means that $\mathfrak{K}$ and its orthogonal complement $\mathfrak{K}^\perp$ are invariant for T and the domain of the operator T splits as

$$\mathrm{Dom}(T) = \big(\mathrm{Dom}(T) \cap \mathfrak{K}\big) \oplus \big(\mathrm{Dom}(T) \cap \mathfrak{K}^\perp\big).$$

Next, we introduce the corresponding notion for sesquilinear forms.

Definition 3.1. We say that a closed subspace $\mathfrak{K}$ of a Hilbert space $\mathcal{H}$ reduces a symmetric densely defined quadratic form $\mathfrak{t}$ with domain $\mathrm{Dom}[\mathfrak{t}] \subseteq \mathcal{H}$ if

(i) $Q\,(\mathrm{Dom}[\mathfrak{t}]) \subseteq \mathrm{Dom}[\mathfrak{t}]$
and
(ii) $\mathfrak{t}[Qu, v] = \mathfrak{t}[u, Qv]$ for all $u, v \in \mathrm{Dom}[\mathfrak{t}]$,

where Q is the orthogonal projection onto $\mathfrak{K}$.

A short computation shows that a closed subspace $\mathfrak{K}$ reduces a symmetric densely defined quadratic form $\mathfrak{t}$ if and only if

$$Q\,(\mathrm{Dom}[\mathfrak{t}]) \subseteq \mathrm{Dom}[\mathfrak{t}] \quad \text{and} \quad \mathfrak{t}[Q^\perp u, Qv] = 0 \ \text{ for all } u, v \in \mathrm{Dom}[\mathfrak{t}]. \tag{3.1}$$

In particular, $\mathfrak{K}$ reduces the form $\mathfrak{b}$ if and only if the orthogonal complement $\mathfrak{K}^\perp$ does.

Taking this into account, along with saying that a closed subspace $\mathfrak{K}$ reduces a form, we also occasionally say that the orthogonal decomposition $\mathcal{H} = \mathfrak{K} \oplus \mathfrak{K}^\perp$ reduces the form.

The following lemma shows that under the domain stability condition, the concepts of reducibility for the form and the associated (representing) self-adjoint operator coincide.

Lemma 3.2. *Assume that $\mathfrak{b}$ is a saddle point form with respect to the decomposition $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$ and let B be the associated operator. Suppose that the domain stability condition* (2.6) *holds.*

Then a closed subspace $\mathfrak{K}$ reduces the form $\mathfrak{b}$ if and only if $\mathfrak{K}$ reduces the operator B.

Proof. Assume that $\mathfrak{K}$ reduces the form $\mathfrak{b}$. Denote by Q the orthogonal projector onto $\mathfrak{K}$. In this case,

$$\mathrm{Dom}[\mathfrak{b}] = \mathrm{Dom}[\mathfrak{a}] = \mathrm{Dom}(|B|^{1/2})$$

and

$$Q\left(\mathrm{Dom}(|B|^{1/2})\right) \subseteq \mathrm{Dom}(|B|^{1/2}).$$

Moreover,

$$\mathfrak{b}[Qx, y] = \mathfrak{b}[x, Qy] \quad \text{for all } x, y \in \mathrm{Dom}[\mathfrak{b}].$$

Since the form $\mathfrak{b}$ is represented by B, we have for all $x, y \in \mathrm{Dom}(|B|^{1/2})$ that

$$\langle |B|^{1/2}Qx, \mathrm{sign}(B)|B|^{1/2}y\rangle = \langle |B|^{1/2}x, \mathrm{sign}(B)|B|^{1/2}Qy\rangle.$$

In particular,

$$\langle Qx, By\rangle = \langle Bx, Qy\rangle \quad \text{for all } x, y \in \mathrm{Dom}(B).$$

Since B is self-adjoint, this means that $Qy \in \mathrm{Dom}(B)$ and that

$$QBy = BQy \quad \text{for all } \ x \in \mathrm{Dom}(B),$$

which shows that $\mathfrak{K}$ reduces the self-adjoint operator B.

To prove the converse, suppose that $\mathfrak{K}$ reduces the operator B. By [42, Satz 8.23], the decomposition also reduces both operators $|B|^{1/2}$ and $\mathrm{sign}(B)$. Together with

$$\mathrm{Dom}[\mathfrak{b}] = \mathrm{Dom}[\mathfrak{a}] = \mathrm{Dom}(|B|^{1/2})$$

this means that

$$Q\,(\mathrm{Dom}[\mathfrak{b}]) \subseteq \mathrm{Dom}[\mathfrak{b}]$$

and that Q commutes with $\mathrm{sign}(B)$ and $|B|^{1/2}$. Thus,

$$\mathfrak{b}[Qu, v] = \langle |B|^{1/2}Qu, \mathrm{sign}(B)|B|^{1/2}v\rangle = \langle |B|^{1/2}u, \mathrm{sign}(B)|B|^{1/2}Qv\rangle = \mathfrak{b}[u, Qv],$$

which shows that $\mathfrak{K}$ reduces the form $\mathfrak{b}$. □

The theorem below generalizes of a series of results of [1, 2, 24, 37], cf. [40, Sect. 2.7], and provides a canonical example of a semi-definite reducing subspace for a saddle point form.

Theorem 3.3. *Let $\mathfrak{b}$ be a saddle point form with respect to the orthogonal decomposition $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$ and B the associated operator. Assume that the form $\mathfrak{b}$ satisfies the domain stability condition* (2.6).

Then the subspace $\mathrm{Ker}(B) \cap \mathcal{H}_+$ reduces both the form $\mathfrak{b}$ and the operator B. In particular, the kernel of B splits as

$$\mathrm{Ker}(B) = (\mathrm{Ker}(B) \cap \mathcal{H}_+) \oplus (\mathrm{Ker}(B) \cap \mathcal{H}_-)\,,$$

the semi-definite subspaces

$$\mathcal{L}_\pm = (\mathrm{Ran}\,\mathsf{E}_B((\mathbb{R}_\pm) \setminus \{0\})) \oplus \left(\mathrm{Ker}(B) \cap \mathcal{H}_\pm\right)$$

are complimentary, and the orthogonal decomposition

$$\mathcal{H} = \mathcal{L}_+ \oplus \mathcal{L}_-$$

reduces both the form $\mathfrak{b}$ and the associated operator B.

Moreover, the subspace $\mathcal{L}_+$ is a graph of a linear contraction $X\colon \mathcal{H}_+ \to \mathcal{H}_-$.

Proof. Assume temporarily that $\mathrm{Ker}(B) = \{0\}$. Then $\mathcal{L}_+$ and $\mathcal{L}_-$ are spectral subspaces and reduce the operator B and, by the domain stability condition and Lemma 3.2, the form $\mathfrak{b}$ as well.

To complete the proof under the assumption $\mathrm{Ker}(B) = \{0\}$, we check that $\mathcal{L}_\pm$ are graph subspaces. Denote by P the orthogonal projection onto $\mathcal{H}_+$ and let

$Q = \mathsf{E}_B(\mathbb{R}_+)$ be the spectral projection of B onto its positive subspace. Introducing the sequence of self-adjoint operators

$$B_n = B + \frac{1}{n}J, \quad J = \begin{pmatrix} I_{\mathcal{H}_+} & 0 \\ 0 & -I_{\mathcal{H}_-} \end{pmatrix}, \quad n \in \mathbb{N},$$

one observes that

$$\lim_{n\to\infty} B_n\varphi = B\varphi, \quad \varphi \in \mathrm{Dom}(B).$$

By [35, Theorem VIII.25], the sequence of operators B_n converges to B in the strong resolvent sense, and therefore, by [35, Theorem VIII.24],

$$\operatorname*{s-lim}_{n\to\infty} \mathsf{E}_{B_n}(\mathbb{R}_+) = \mathsf{E}_B(\mathbb{R}_+), \tag{3.2}$$

since 0 is not an eigenvalue of B.

Taking into account that the operator B_n is associated with the form $\mathfrak{b}_n$ given by

$$\mathfrak{b}_n[x, y] := \mathfrak{b}[x, y] + \frac{1}{n}\langle x, Jy\rangle$$

and that the interval $(-1/n, 1/n)$ belongs to its resolvent set, one applies the Tan 2Θ-Theorem [19, Theorem 3.1] to conclude that

$$\|Q - \mathsf{E}_{B_n}(\mathbb{R}_+)\| < \frac{\sqrt{2}}{2}. \tag{3.3}$$

Since (3.2) holds, one also gets the weak limit

$$\operatorname*{w-lim}_{n\to\infty}(Q - \mathsf{E}_{B_n}(\mathbb{R}_+)) = Q - \mathsf{E}_B(\mathbb{R}_+). \tag{3.4}$$

Using the principle of uniform boundedness, see [21, Eq. (3.2), Chap. III], from (3.3) and (3.4) one obtains the bound

$$\|Q - \mathsf{E}_B(\mathbb{R}_+)\| \le \liminf_{n\to\infty} \|Q - \mathsf{E}_{B_n}(\mathbb{R}_+)\| \le \frac{\sqrt{2}}{2}.$$

Hence, $\mathcal{L}_+$ is the graph subspace $\mathrm{Graph}(\mathcal{H}_+, X)$ with X being a contraction, see [22, Corollary 3.4]. The orthogonal complement $\mathcal{L}_-$ is then the graph subspace $\mathrm{Graph}(\mathcal{H}_-, -X^*)$.

We now treat the general case (of a non-trivial kernel).

First, we check that the semi-positive subspaces $\mathcal{L}_\pm$ reduce the operator B, and thus also the form $\mathfrak{b}$.

It is clear that both $\mathcal{L}_\pm$ are invariant for B. It is also clear that the subspaces $\mathcal{L}_\pm$ are complimentary if and only if the kernel splits as

$$\mathrm{Ker}(B) = (\mathrm{Ker}(B) \cap \mathcal{H}_+) \oplus (\mathrm{Ker}(B) \cap \mathcal{H}_-). \tag{3.5}$$

To prove (3.5), recall (see [37, Theorem 2.13]) that the kernel of B can be represented as

$$\mathrm{Ker}(B) = (\mathrm{Ker}(A_+) \cap \mathcal{K}_+) \oplus (\mathrm{Ker}(A_-) \cap \mathcal{K}_-), \tag{3.6}$$

where $A_\pm$ are self-adjoint non-negative operators associated with the forms $\mathfrak{a}_\pm$ and the subspaces $\mathcal{K}_+$ and $\mathcal{K}_-$ are given by

$$\mathcal{K}_\pm := \big\{x_\pm \in \mathrm{Dom}[\mathfrak{a}_\pm] \mid \mathfrak{v}[x_+, x_-] = 0 \quad \text{for all } x_\mp \in \mathrm{Dom}[\mathfrak{a}_\mp]\big\} \subseteq \mathcal{H}_\pm.$$

Hence $\mathrm{Ker}(B) \cap \mathcal{H}_\pm = \mathrm{Ker}(A_\pm) \cap \mathcal{K}_\pm$ and (3.5) follows.

Next, in view of (3.5), since $\mathcal{H}$ naturally splits as

$$\mathcal{H} = \mathrm{Ran}\,\mathsf{E}_B(\mathbb{R}_+) \oplus \mathrm{Ker}(B) \oplus \mathrm{Ran}\,\mathsf{E}_B(\mathbb{R}_-),$$

one gets

$$\begin{aligned}\mathrm{Dom}(B) = \big(\mathrm{Dom}(B) \cap \mathrm{Ran}\,\mathsf{E}_B(\mathbb{R}_+)\big) \oplus (\mathrm{Ker}(B) \cap \mathcal{H}_+)\\ \oplus (\mathrm{Ker}(B) \cap \mathcal{H}_-) \oplus \big(\mathrm{Dom}(B) \cap \mathrm{Ran}\,\mathsf{E}_B(\mathbb{R}_+)\big).\end{aligned}$$

This representation shows that the domain $\mathrm{Dom}(B)$ splits as

$$\mathrm{Dom}(B) = \big(\mathrm{Dom}(B) \cap \mathcal{L}_+\big) \oplus \big(\mathrm{Dom}(B) \cap \mathcal{L}_-\big). \tag{3.7}$$

Summing up, we have shown that $\mathcal{L}_\pm$ are B-invariant mutually orthogonal subspaces such that (3.7) holds. That is, the subspaces $\mathcal{L}_\pm$ reduce the operator B and therefore the form $\mathfrak{b}$.

To complete the proof, we now need to check that $\mathcal{L}_+$ (and thus also $\mathcal{L}_-$) is a graph subspace with a contractive angular operator.

By [22, Corollary 3.4], it it sufficient to show that

$$\|Q - P\| \le \frac{\sqrt{2}}{2}, \tag{3.8}$$

where Q and P are the orthogonal projection onto $\mathcal{H}_+$ and $\mathcal{L}_+$, respectively.

We will prove (3.8) by reducing the problem to the one where the kernel is trivial.

First we show that $\mathrm{Ker}(B)$ reduces the operator A. Indeed, by (3.6) we have $\mathrm{Ker}(B) \subseteq \mathrm{Ker}(A)$, so that $\mathrm{Ker}(B)$ is invariant for A. Hence, $\mathrm{Ker}(B)^\perp$ is invariant for A as well. It remains to check that $\mathrm{Dom}(A)$ splits as

$$\mathrm{Dom}(A) = (\mathrm{Dom}(A) \cap \mathrm{Ker}(B)) \oplus (\mathrm{Dom}(A) \cap \mathrm{Ker}(B)^\perp). \tag{3.9}$$

Indeed, since $\mathrm{Ker}(B)$ reduces B, by [42, Satz 8.23], the subspace $\mathrm{Ker}(B)$ also reduces $|B|^{1/2}$. By the required domain stability condition, this implies that $\mathrm{Ker}(B)$ reduces $|A|^{1/2}$ and, by [42, Satz 8.23] again, also $|A|$. Thus (3.9) holds by observing that $\mathrm{Dom}(A) = \mathrm{Dom}(|A|)$.

We now complete the proof that $\mathcal{L}_+ = \mathrm{Graph}(\mathcal{H}_+, X)$ is a graph subspace for a contraction X.

Taking into account that the subspace $\widetilde{\mathcal{H}} := \mathrm{Ker}(B)^\perp$ reduces both A and B, denote by $\widetilde{A} := A|_{\widetilde{\mathcal{H}}}$ and $\widetilde{B} := (B)|_{\widetilde{\mathcal{H}}}$ the corresponding parts of A and B, respectively. In particular, $\widetilde{A}$ and $\widetilde{B}$ are self-adjoint operators and $\mathrm{Ker}(\widetilde{B}) = \{0\}$.

In view of the kernel splitting (3.6), a simple reasoning shows that $\widetilde{\mathcal{H}}$ splits as

$$\widetilde{\mathcal{H}} = \widetilde{\mathcal{H}}_+ \oplus \widetilde{\mathcal{H}}_- \quad \text{with} \quad \widetilde{\mathcal{H}}_+ := \mathcal{H}_+ \cap \widetilde{\mathcal{H}} \quad \text{and} \quad \widetilde{\mathcal{H}}_- := \mathcal{H}_- \cap \widetilde{\mathcal{H}}\,,$$

and that the operator $\widetilde{A}$ is represented as the diagonal block matrix

$$\widetilde{A} = \begin{pmatrix} \widetilde{A}_+ & 0 \\ 0 & -\widetilde{A}_- \end{pmatrix}_{\widetilde{\mathcal{H}}_+ \oplus \widetilde{\mathcal{H}}_-}$$

with

$$\sup \operatorname{spec}(-\widetilde{A}_-) \le 0 \le \inf \operatorname{spec}(\widetilde{A}_+)\,.$$

In this case the corresponding sesquilinear symmetric form $\widetilde{\mathfrak{a}}$ also splits into the difference of two non-negative forms. The restriction $\widetilde{\mathfrak{b}} = \mathfrak{b}|_{\widetilde{\mathcal{H}}}$ is clearly seen to be a saddle point form associated with the self-adjoint operator $\widetilde{B}$. Since $\operatorname{Ker}(\widetilde{B}) = \{0\}$, by the above reasoning, we get the inequality

$$\|\widetilde{Q} - \mathsf{E}_{\widetilde{B}}(\mathbb{R}_+)\| \le \frac{\sqrt{2}}{2},$$

where $\widetilde{Q}$ is the orthogonal projection onto $\widetilde{\mathcal{H}}_+$ and $\mathsf{E}_{\widetilde{B}}(\mathbb{R}_+)$ is the spectral projection of $\widetilde{B}$ for the positive part. In particular, as in the previous case, $\operatorname{Ran} \mathsf{E}_{\widetilde{B}}(\mathbb{R}_+) = \operatorname{Graph}(\widetilde{\mathcal{H}}_+, \widetilde{X})$ is the graph of a linear contraction $\widetilde{X} \colon \widetilde{\mathcal{H}}_+ \to \widetilde{\mathcal{H}}_-$.

Denoting by X the extension of the operator $\widetilde{X}$ by zero on $\operatorname{Ker}(B) \cap \mathcal{H}_+$ and taking into account that by (3.6)

$$A|_{\operatorname{Ker}(B)\cap\mathcal{H}_+} = B|_{\operatorname{Ker}(B)\cap\mathcal{H}_+} = 0,$$

we obviously get that $\mathcal{L}_+ = \operatorname{Graph}(\mathcal{H}_+, X)$. Observing that the extended operator X is also a contraction completes the proof. □

4. Regular embeddings and direct rotations

Given the orthogonal decomposition

$$\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-,$$

suppose that Hilbert spaces $\dot{\mathcal{H}}_\pm$ are continuously embedded in $\mathcal{H}_\pm$,

$$\dot{\mathcal{H}}_\pm \hookrightarrow \mathcal{H}_\pm, \tag{4.1}$$

so that their direct sum $\dot{\mathcal{H}} = \dot{\mathcal{H}}_+ \oplus \dot{\mathcal{H}}_-$ is also continuously embedded in $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$.

Suppose that a subspace $\mathcal{G}_+$ can be represented as a graph of a bounded operator X from $\mathcal{H}_+$ to $\mathcal{H}_-$ and let

$$\mathcal{H} = \mathcal{G}_+ \oplus \mathcal{G}_- \tag{4.2}$$

be the corresponding decomposition with $\mathcal{G}_- = (\mathcal{G}_+)^\perp$, the graph of the bounded operator $-X^* \colon \mathcal{H}_- \to \mathcal{H}_+$.

Definition 4.1. We say that the graph decomposition (4.2) is $\dot{\mathcal{H}}$-regular (with respect to the embedding) if the linear sets

$$\dot{\mathcal{G}}_\pm = \mathcal{G}_\pm \cap \dot{\mathcal{H}}$$

naturally embedded in $\dot{\mathcal{H}}$ are closed complimentary graph subspaces in the Hilbert space $\dot{\mathcal{H}}$ with respect to the decomposition $\dot{\mathcal{H}} = \dot{\mathcal{H}}_+ \oplus \dot{\mathcal{H}}_-$.

Denote by P and Q the orthogonal projections onto the subspaces $\mathcal{H}_+$ and $\mathcal{G}_+$, respectively.

Recall that as long as it is known that $\mathcal{G}_+$ is a graph subspace, there exists a unique unitary operator U on $\mathcal{H}$ that maps $\mathcal{H}_+$ to $\mathcal{G}_+$, such that

$$UP = QU,$$

the diagonal entries of which (in its block matrix representation with respect to the decomposition $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$) are non-negative operators, see [8]. In this case the operator U is called the direct rotation from the subspace $\mathcal{H}_+ = \mathrm{Ran}(P)$ to the subspace $\mathcal{G}_+ = \mathrm{Ran}(Q)$.

Lemma 4.2. *Suppose that the graph decomposition* (4.2) *is $\dot{\mathcal{H}}$-regular with respect to the embedding* (4.1)*. Let U and $\dot{U}$ be the direct rotation from $\mathcal{H}_+$ to $\mathcal{G}_+$ in the space $\mathcal{H}$ and from $\dot{\mathcal{H}}_+$ to $\dot{\mathcal{G}}_+$ in $\dot{\mathcal{H}}$, respectively. Then*

$$\dot{U} = U|_{\dot{\mathcal{H}}}\,.$$

Proof. Since the graph decomposition (4.2) is $\dot{\mathcal{H}}$-regular, it follows that $\mathcal{G}_+ \cap \dot{\mathcal{H}}$ is the graph of a bounded operator $\dot{X} : \dot{\mathcal{H}}_+ \to \dot{\mathcal{H}}_-$. Therefore, $\mathcal{G}_+ \cap \dot{\mathcal{H}}$ is the graph of $-\dot{X}^*$. Clearly,

$$\dot{X} = X|_{\dot{\mathcal{H}}_+} \quad \text{and} \quad (-\dot{X}^*) = (-X^*)|_{\dot{\mathcal{H}}_-}.$$

In particular,

$$X^*X|_{\mathcal{H}_+} = \dot{X}^*\dot{X} \quad \text{and} \quad XX^*|_{\mathcal{H}_-} = \dot{X}\dot{X}^*.$$

A classic Neumann series argument shows that

$$(tI + X^*X)^{-1}|_{\mathcal{H}_+} = (tI + \dot{X}^*\dot{X})^{-1} \tag{4.3}$$

for $|t|$ is large enough. Taking into account the continuity of the embedding, one extends (4.3) for all $t > 0$ by analytic continuation. Next, using the formula for the fractional power (see, e.g., [21, Ch. V, eq. (3.53)])

$$T^{-1/2} = \frac{1}{\pi}\int_0^\infty t^{-1/2}(T + tI)^{-1}dt$$

valid for any positive self-adjoint operator T and taking $T = (I + X^*X)|_{\mathcal{H}_+}$ first and then $T = I + \dot{X}^*\dot{X}$ in the Hilbert spaces $\mathcal{H}_+$ and $\mathcal{H}$, respectively, from (4.3) one deduces that

$$(I + \dot{X}^*\dot{X})^{-1/2}|_{\mathcal{H}_+} = (I + \dot{X}^*\dot{X})^{-1/2}. \tag{4.4}$$

Analogously,

$$(I + XX^*)^{-1/2}|_{\mathcal{H}_-} = (I + \dot{X}\dot{X}^*)^{-1/2}. \tag{4.5}$$

Since the direct rotation U admits the representation

$$U = \begin{pmatrix} (I+X^*X)^{-1/2} & -X^*(I+XX^*)^{-1/2} \\ X(I+X^*X)^{-1/2} & (I+XX^*)^{-1/2} \end{pmatrix},$$

cf. [3, 8, 22], see also [39, Proof of Proposition 3.3], and analogously

$$\dot{U} = \begin{pmatrix} (I+\dot{X}^*\dot{X})^{-1/2} & -\dot{X}^*(I+\dot{X}\dot{X}^*)^{-1/2} \\ \dot{X}(I+\dot{X}^*\dot{X})^{-1/2} & (I+\dot{X}\dot{X}^*)^{-1/2} \end{pmatrix},$$

the assertion follows from (4.4) and (4.5). □

Remark 4.3. If $\mathcal{G}_+$ is the graph of a bounded operator X from $\mathcal{H}_+$ to $\mathcal{H}_-$, introduce

$$Y = \begin{pmatrix} 0 & -X^* \\ X & 0 \end{pmatrix}_{\mathcal{H}_+\oplus\mathcal{H}_-}.$$

Then the direct rotation U is just the unitary operator from the polar decomposition of the operator $I+Y$,

$$(I+Y) = U|I+Y|.$$

Observe that the $\dot{\mathcal{H}}$-regularity of the decomposition

$$\mathcal{H} = \mathrm{Graph}(\mathcal{H}_+, X) \oplus \mathrm{Graph}(\mathcal{H}_-, -X^*)$$

can equivalently be reformulated in purely algebraic terms that invoke mapping properties of the operators $I \pm Y$ only. That is, the graph space decomposition (4.2) is $\dot{\mathcal{H}}$-regular if and only if the operators $I \pm Y$ are algebraic/ topologic automorphisms of $\dot{\mathcal{H}}$, see [30, Lemma 3.1, Remark 3.2].

5. Block-diagonalization of associated operators by a direct rotation

From now and later on, given a saddle point form $\mathfrak{b}$, denote by $\mathcal{H}^1_A$ the space $\mathrm{Dom}[\mathfrak{b}]$ equipped with the graph norm of the operator $|A|^{1/2}$, where A is the diagonal self-adjoint operator associated with the diagonal part $\mathfrak{a}$ of the form $\mathfrak{b}$ (see eq. (2.4)).

One of the main results of the current paper is as follows.

Theorem 5.1. *Let $\mathfrak{b}$ be a saddle point form with respect to the orthogonal decomposition $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$ and B the associated operator. Assume that the form $\mathfrak{b}$ satisfies the domain stability condition* (2.6)*.*

Suppose that the decomposition

$$\mathcal{H} = \mathcal{L}_+ \oplus \mathcal{L}_- \tag{5.1}$$

referred to in Theorem 3.3 *is $\mathcal{H}^1_A$-regular, where A is the diagonal self-adjoint operator given by* (2.4) *and associated with the diagonal part $\mathfrak{a}$ of the form $\mathfrak{b}$.*

Then the form $\mathfrak{b}$ *and the associated operator* B *can be block diagonalized by the direct rotation* U *from the subspace* $\mathcal{H}_+$ *to the reducing graph subspace* $\mathcal{L}_+$*. That is,*

(i) *the form*

$$\widehat{\mathfrak{b}}[f,g] = \mathfrak{b}[Uf,Ug], \quad f,g \in \mathrm{Dom}[\widehat{\mathfrak{b}}] = \mathrm{Dom}[\mathfrak{b}]$$

is a diagonal saddle point form with respect to the decomposition $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$*,*

$$\widehat{\mathfrak{b}} = \widehat{\mathfrak{b}}_+ \oplus (-\widehat{\mathfrak{b}}_-),$$

with $\widehat{\mathfrak{b}}_\pm = \pm\widehat{\mathfrak{b}}|_{\mathcal{H}_\pm}$*. In particular, the non-negative forms* $\widehat{\mathfrak{b}}_\pm$ *are closed;*

(ii) *the associated operator* $\widehat{B}$ *can be represented as the diagonal operator matrix,*

$$\widehat{B} = U^*BU = \begin{pmatrix} \widehat{B}_+ & 0 \\ 0 & -\widehat{B}_- \end{pmatrix}_{\mathcal{H}_+\oplus\mathcal{H}_-};$$

(iii) *the non-negative closed forms* $\widehat{\mathfrak{b}}_\pm$ *are in one-to-one correspondence to the non-negative self-adjoint operators* $\widehat{B}_\pm$*.*

If, in addition, the form $\mathfrak{b}$ *is semi-bounded, then the hypotheses that* $\mathfrak{b}$ *satisfies the domain stability condition and that the decomposition* (5.1) *is regular are redundant.*

Proof. Since the domain stability condition (2.6) implies that the Hilbert spaces $\mathcal{H}_A^1$ and $\mathcal{H}_B^1$ coincide as the sets and therefore have the same topology, the form $\mathfrak{b}$ can be represented by a bounded operator $\mathcal{B}$ as

$$\mathfrak{b}[x,y] = \langle x, \mathcal{B}y\rangle_{\mathcal{H}_A^1}, \quad x,y \in \mathrm{Dom}[\mathfrak{b}]. \tag{5.2}$$

Let $\dot{U}$ denote the direct rotation from $\mathcal{H}_+\cap\mathcal{H}_A^1$ to $\mathcal{L}_+\cap\mathcal{H}_A^1$ in $\mathcal{H}_A^1$. By Lemma 4.2 one has $\dot{U} = U|_{\mathcal{H}_A^1}$ and therefore

$$\mathfrak{b}[Ux,Uy] = \langle \dot{U}x, \mathcal{B}\dot{U}y\rangle_{\mathcal{H}_A^1} = \langle x, (\dot{U})^*\mathcal{B}\dot{U}y\rangle_{\mathcal{H}_A^1}.$$

Since the decomposition (5.1) reduces $\mathfrak{b}$, it follows that $(\dot{U})^*\mathcal{B}\dot{U}$ is a diagonal operator matrix in $\mathcal{H}_A^1$ with respect to the decomposition $\mathcal{H}_A^1 = \big(\mathcal{H}_+\cap\mathcal{H}_A^1\big)\oplus\big(\mathcal{H}_-\cap\mathcal{H}_A^1\big)$. The corresponding subspaces $\mathcal{L}_\pm$ are non-negative subspaces for the operator B, so that

$$(\dot{U})^*\mathcal{B}\dot{U} = \begin{pmatrix} \mathcal{B}_+ & 0 \\ 0 & -\mathcal{B}_- \end{pmatrix}_{(\mathcal{H}_+\cap\mathcal{H}_A^1)\oplus(\mathcal{H}_-\cap\mathcal{H}_A^1)},$$

where $\mathcal{B}_\pm$ are non-negative bounded operators in $\mathcal{H}_\pm\cap\mathcal{H}_A^1$. Since

$$\mathfrak{b}[Ux_\pm, Uy_\pm] = \pm\langle x_\pm, \mathcal{B}_\pm y_\pm\rangle_{\mathcal{H}_A^1\cap\mathcal{H}_\pm},$$

one observes that $\mathfrak{b}[Ux_\pm, Uy_\pm]$, $x_\pm, y_\pm \in \mathcal{H}_\pm\cap\mathcal{H}_A^1$ defines a sign-definite closed form on $\mathcal{H}_\pm\cap\mathcal{H}_A^1$. This proves (i).

On the other hand,

$$\mathfrak{b}[Ux, Uy] = \langle x, U^*BUy\rangle_{\mathcal{H}}, \quad x \in \mathrm{Dom}[\mathfrak{b}], \quad y \in U^{-1}(\mathrm{Dom}(B)).$$

In particular, one has

$$\mathfrak{b}[Ux_\pm, Uy_\pm] = \langle x_\pm, \pm\widehat{B}_\pm y_\pm\rangle_{\mathcal{H}}, \quad x_\pm \in \mathrm{Dom}[\mathfrak{a}_\pm], \quad y_\pm \in U^{-1}(\mathrm{Dom}(B)) \cap \mathcal{H}_\pm, \tag{5.3}$$

which shows (ii).

The assertion (iii) now follows from (i) and (5.3).

Next, we prove the last assertion of the theorem.

Denote by Q the orthogonal projection onto the subspace $\mathcal{L}_+$. Then

$$Q = \begin{pmatrix} (I_{\mathcal{H}_+} + X^*X)^{-1} & (I_{\mathcal{H}_+} + X^*X)^{-1}X^* \\ X(I_{\mathcal{H}_+} + X^*X)^{-1} & X(I_{\mathcal{H}_+} + X^*X)^{-1}X^* \end{pmatrix} \tag{5.4}$$

and

$$Q^\perp = \begin{pmatrix} X^*(I_{\mathcal{H}_-} + XX^*)^{-1}X & -X^*(I_{\mathcal{H}_-} + XX^*)^{-1} \\ -(I_{\mathcal{H}_-} + XX^*)^{-1}X & (I_{\mathcal{H}_-} + XX^*)^{-1} \end{pmatrix}. \tag{5.5}$$

Note that since the subspace $\mathcal{L}_+$ reduces the form $\mathfrak{b}$, both Q and $Q^\perp$ map $\mathrm{Dom}[\mathfrak{b}]$ into itself. In particular, $(I_{\mathcal{H}_+} + X^*X)^{-1}$ maps $\mathcal{H}_- \cap \mathrm{Dom}[\mathfrak{b}]$ into itself.

Now, since the form $\mathfrak{b}$ is semibounded from below, the operator $I + XX^*$ is bijective on $\mathcal{H}_- \cap \mathrm{Dom}[\mathfrak{b}]$. Therefore, the operator

$$(I - Y^2)^{-1} = \begin{pmatrix} (I_{\mathcal{H}_+} + X^*X)^{-1} & 0 \\ 0 & (I_{\mathcal{H}_-} + XX^*)^{-1} \end{pmatrix}$$

maps $\mathrm{Dom}[\mathfrak{b}]$ into itself.

Again, since $I+XX^*$ is bijective on $\mathcal{H}_- = \mathrm{Dom}[\mathfrak{b}]\cap\mathcal{H}_-$ and $Q^\perp$ maps $\mathrm{Dom}[\mathfrak{b}]$ into itself, it follows from (5.5) that X maps $\mathrm{Dom}[\mathfrak{b}] \cap \mathcal{H}_+$ into $\mathrm{Dom}[\mathfrak{b}] \cap \mathcal{H}_-$ and that X^* maps $\mathrm{Dom}[\mathfrak{b}] \cap \mathcal{H}_-$ into $\mathrm{Dom}[\mathfrak{b}] \cap \mathcal{H}_+$. Thus, Y leaves the form domain $\mathrm{Dom}[\mathfrak{b}]$ invariant and so do the operators $I + Y$, $I - Y$ and $I - Y^2$.

Summing up, both $(I - Y^2)$ and $(I - Y^2)^{-1}$ map $\mathrm{Dom}[\mathfrak{b}]$ into itself. That is, the restriction of the map

$$I - Y^2 = (I - Y)(I + Y)$$

on $\mathrm{Dom}[\mathfrak{b}]$ is bijective on $\mathrm{Dom}[\mathfrak{b}]$. In particular $I + Y$ is bijective on $\mathrm{Dom}[\mathfrak{b}]$ and by Remark 4.3 the decomposition $\mathcal{H} = \mathcal{L}_+ \oplus \mathcal{L}_-$ is $\mathcal{H}^1_A$-regular, which completes the proof. □

6. The Riccati equation

The existence of a reducing graph subspace for a saddle point form, as, e.g., in Theorem 5.1, is closely related to the solvability of the associated block form Riccati equation.

Hypothesis 6.1. Suppose that $\mathfrak{b}$ is a saddle point form with respect to the decomposition $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$. Assume that a subspace $\mathcal{G}_+$ is the graph of a bounded operator $X : \mathcal{H}_+ \to \mathcal{H}_-$ and that Y is the skew-symmetric off-diagonal operator Y

$$Y = \begin{pmatrix} 0 & -X^* \\ X & 0 \end{pmatrix}_{\mathcal{H}_+ \oplus \mathcal{H}_-}.$$

Theorem 6.2. *Assume Hypothesis* 6.1. *Assume, in addition, that the orthogonal decomposition $\mathcal{H} = \mathcal{G}_+ \oplus \mathcal{G}_-$, with $\mathcal{G}_- = \mathcal{G}_+^\perp$, is $\mathcal{H}_A^1$-regular.*

Then the decomposition $\mathcal{H} = \mathcal{G}_+ \oplus \mathcal{G}_-$ reduces the form $\mathfrak{b}$ if and only if the skew-symmetric off-diagonal operator Y is a solution to the block form Riccati equation

$$\mathfrak{a}[f, Yg] + \mathfrak{a}[Yf, g] + \mathfrak{v}[Yf, Yg] + \mathfrak{v}[f, g] = 0, \quad f, g \in \mathrm{Dom}[\mathfrak{a}], \tag{6.1}$$

$$\mathrm{Ran}(Y|_{\mathrm{Dom}[\mathfrak{a}]}) \subseteq \mathrm{Dom}[\mathfrak{a}].$$

Proof. The proof of this theorem is a direct combination of the following two lemmas. □

Lemma 6.3. *Assume Hypothesis* 6.1. *Suppose that the orthogonal decomposition $\mathcal{H} = \mathcal{G}_+ \oplus \mathcal{G}_-$, with $\mathcal{G}_- = \mathcal{G}_+^\perp$, reduces $\mathfrak{b}$.*

If the space $\mathcal{H}_A^1$ is Y-invariant, then Y is a solution to the block-form Riccati equation (6.1)*.*

Proof. Assume that the decomposition reduces $\mathfrak{b}$. Since $\mathrm{Dom}[\mathfrak{b}] = \mathrm{Dom}[\mathfrak{a}] = \mathcal{H}_A^1$ (as a set), the Y-invariance of $\mathcal{H}_A^1$ implies that X and X^* map $\mathrm{Dom}[\mathfrak{a}_+] = \mathrm{Dom}(A_+^{1/2})$ into $\mathrm{Dom}[\mathfrak{a}_-] = \mathrm{Dom}(A_-^{1/2})$, and vice versa, respectively. Denote by Q the orthogonal projection onto $\mathcal{G}(\mathcal{H}_+, X)$. By (3.1), we have

$$0 = \mathfrak{b}[Q^\perp(-X^*y \oplus y), Q(x \oplus Xx)] = \mathfrak{b}[-X^*y \oplus y, x \oplus Xx], \tag{6.2}$$

$$x \in \mathrm{Dom}[\mathfrak{a}_+],\ y \in \mathrm{Dom}[\mathfrak{a}_-].$$

Taking into account that $\mathfrak{b} = \mathfrak{a} + \mathfrak{v}$, where $\mathfrak{a}$ and $\mathfrak{v}$ are the diagonal and off-diagonal parts, respectively, and that $\mathfrak{a} = \mathfrak{a}_+ \oplus (-\mathfrak{a}_-)$, the equality (6.2) shows that X is a solution to the Riccati equation

$$\mathfrak{a}_+[-X^*y, x] - \mathfrak{a}_-[y, Xx] + \mathfrak{v}[-X^*y, Xx] + \mathfrak{v}[y, x] = 0, \tag{6.3}$$

$$x \in \mathrm{Dom}[\mathfrak{a}_+], \quad y \in \mathrm{Dom}[\mathfrak{a}_-].$$

Set

$$f = x_+ \oplus x_-,\ g = y_+ \oplus y_-, \quad x_\pm,\ y_\pm \in \mathrm{Dom}[\mathfrak{a}_\pm],$$

combine the Riccati equation (6.3) with $x = y_+,\ y = x_-$ plugged in, and the complex conjugate of (6.3) with $x = x_+,\ y = y_-$ plugged in, to get

$$\begin{aligned}
&\mathfrak{a}[f, Yg] + \mathfrak{a}[Yf, g] + \mathfrak{v}[Yf, Yg] + \mathfrak{v}[f, g] \\
&\quad = \mathfrak{a}\left[\begin{pmatrix} x_+ \\ x_- \end{pmatrix}, \begin{pmatrix} 0 & -X^* \\ X & 0 \end{pmatrix}\begin{pmatrix} y_+ \\ y_- \end{pmatrix}\right] + \mathfrak{a}\left[\begin{pmatrix} 0 & -X^* \\ X & 0 \end{pmatrix}\begin{pmatrix} x_+ \\ x_- \end{pmatrix}, \begin{pmatrix} y_+ \\ y_- \end{pmatrix}\right] \\
&\qquad + \mathfrak{v}\left[\begin{pmatrix} 0 & -X^* \\ X & 0 \end{pmatrix}\begin{pmatrix} x_+ \\ x_- \end{pmatrix}, \begin{pmatrix} 0 & -X^* \\ X & 0 \end{pmatrix}\begin{pmatrix} y_+ \\ y_- \end{pmatrix}\right] + \mathfrak{v}\left[\begin{pmatrix} x_+ \\ x_- \end{pmatrix}, \begin{pmatrix} y_+ \\ y_- \end{pmatrix}\right] \\
&\quad = \mathfrak{a}_+[x_+, -X^*y_-] - \mathfrak{a}_-[x_-, Xy_+] + \mathfrak{a}_+[-X^*x_-, y_+] - \mathfrak{a}_-[Xx_+, y_-] \\
&\qquad + \mathfrak{v}[-X^*x_-, Xy_+] + \mathfrak{v}[Xx_+, -X^*y_-] + \mathfrak{v}[x_+, y_-] + \mathfrak{v}[x_-, y_+] \\
&\quad = \overline{\mathfrak{a}_+[-X^*y_-, x_+] - \mathfrak{a}_-[y_-, Xx_+] + \mathfrak{v}[-X^*y_-, Xx_+] + \mathfrak{v}[y_-, x_+]} \\
&\qquad + \mathfrak{a}_+[-X^*x_-, y_+] - \mathfrak{a}_-[x_-, Xy_+] + \mathfrak{v}[-X^*x_-, Xy_+] + \mathfrak{v}[x_+, y_-] \\
&\quad = 0,
\end{aligned}$$

which shows that Y is a solution of the block Riccati equation (6.1). □

Lemma 6.4. *Assume Hypothesis* 6.1. *Suppose that Y solves the block form Riccati equation* (6.1) *and assume that $\mathcal{H}_A^1 \subseteq \operatorname{Ran}(I - Y)|_{\mathcal{H}_A^1}$.*

Then the orthogonal decomposition $\mathcal{H} = \mathcal{G}_+ \oplus \mathcal{G}_-$, with $\mathcal{G}_- = \mathcal{G}_+^\perp$, reduces the form $\mathfrak{b}$.

Proof. Let Q denote the orthogonal projection onto $\mathcal{G}(\mathcal{H}_+, X)$. Recall that Q is given by the block matrix (5.4)

$$Q = \begin{pmatrix} (I_{\mathcal{H}_+} + X^*X)^{-1} & (I_{\mathcal{H}_+} + X^*X)^{-1}X^* \\ X(I_{\mathcal{H}_+} + X^*X)^{-1} & X(I_{\mathcal{H}_+} + X^*X)^{-1}X^* \end{pmatrix}_{\mathcal{H}_+ \oplus \mathcal{H}_-}. \tag{6.4}$$

By hypothesis, one has that $(I - Y)\operatorname{Dom}[\mathfrak{a}] \supseteq \operatorname{Dom}[\mathfrak{a}]$. Since Y is a solution of the Riccati equation (6.1), then necessarily $(I - Y)\operatorname{Dom}[\mathfrak{a}] \subseteq \operatorname{Dom}[\mathfrak{a}]$. Thus, $I - Y$ is bijective on $\operatorname{Dom}[\mathfrak{a}]$. So is the operator

$$I - Y^2 = (I - Y)J(I - Y)J = \begin{pmatrix} I_{\mathcal{H}_+} + X^*X & 0 \\ 0 & I_{\mathcal{H}_-} + XX^* \end{pmatrix},$$

where the involution J is given by (2.1).

In particular, the operators $I_{\mathcal{H}_+} + X^*X$ and $I_{\mathcal{H}_-} + XX^*$ are bijective on $\operatorname{Dom}[\mathfrak{a}_+]$ and $\operatorname{Dom}[\mathfrak{a}_-]$, respectively. Since $I - Y$ is bijective on $\operatorname{Dom}[\mathfrak{a}]$, one also observes that X maps $\operatorname{Dom}[\mathfrak{a}_+]$ into $\operatorname{Dom}[\mathfrak{a}_-]$ and that X^* maps $\operatorname{Dom}[\mathfrak{a}_-]$ into $\operatorname{Dom}[\mathfrak{a}_+]$. Taking into account the explicit representation (6.4), one concludes that the operator Q maps $\operatorname{Dom}[\mathfrak{b}] = \operatorname{Dom}[\mathfrak{a}]$ into itself.

Therefore, for any $\tilde{y} \in \operatorname{Dom}[\mathfrak{b}]$, there exists an $x \in \operatorname{Dom}[\mathfrak{a}_+]$ such that

$$Q\tilde{y} = x \oplus Xx.$$

Similarly, for any $\tilde{x} \in \operatorname{Dom}[\mathfrak{b}]$ there exists a $y \in \operatorname{Dom}[\mathfrak{a}_-]$ such that

$$Q^\perp \tilde{x} = -X^*y \oplus y.$$

Assuming that $x \in \mathrm{Dom}[\mathfrak{a}_+]$ and $y \in \mathrm{Dom}[\mathfrak{a}_-]$, we have

$$\begin{aligned}
\mathfrak{b}[Q^\perp \tilde{x}, Q\tilde{y}] &= \mathfrak{b}[-X^*y \oplus y, x \oplus Xx] \\
&= \mathfrak{a}[-X^*y \oplus y, x \oplus Xx] + \mathfrak{v}[-X^*y \oplus y, x \oplus Xx] \\
&= \mathfrak{a}_+[-X^*y, x] - \mathfrak{a}_-[y, Xx] + \mathfrak{v}[-X^*y, Xx] + \mathfrak{v}[y, x] \\
&= \mathfrak{a}\left[\begin{pmatrix} x \\ 0 \end{pmatrix}, \begin{pmatrix} 0 & -X^* \\ X & 0 \end{pmatrix}\begin{pmatrix} 0 \\ y \end{pmatrix}\right] + \mathfrak{a}\left[\begin{pmatrix} 0 & -X^* \\ X & 0 \end{pmatrix}\begin{pmatrix} x \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ y \end{pmatrix}\right] \\
&\quad + \mathfrak{v}\left[\begin{pmatrix} 0 & -X^* \\ X & 0 \end{pmatrix}\begin{pmatrix} x \\ 0 \end{pmatrix}, \begin{pmatrix} 0 & -X^* \\ X & 0 \end{pmatrix}\begin{pmatrix} 0 \\ y \end{pmatrix}\right] + \mathfrak{v}\left[\begin{pmatrix} x \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ y \end{pmatrix}\right] \\
&= \mathfrak{a}[f, Yg] + \mathfrak{a}[Yf, g] + \mathfrak{v}[Yf, Yg] + \mathfrak{v}[f, g] \\
&= 0,
\end{aligned}$$

where we have used the block Riccati equation (6.1) for $f = x \oplus 0$ and $g = 0 \oplus y$ on the last step. This implies that

$$\mathfrak{b}[Q^\perp \tilde{x}, Q\tilde{y}] = 0 \quad \text{for all} \quad \tilde{x}, \tilde{y} \in \mathrm{Dom}[\mathfrak{b}],$$

and therefore, the graph subspace $\mathcal{G}_+ = \mathcal{G}(\mathcal{H}_+, X)$ reduces the form $\mathfrak{b}$ (see (3.1)). □

Now we are ready to present a generalization of assertion (i) from Theorem 5.1 that yields the block diagonalization of a saddle point form, provided that the latter has a reducing subspace.

Theorem 6.5. *Assume Hypothesis* 6.1*. Suppose that the graph decomposition $\mathcal{H} = \mathcal{G}_+ \oplus \mathcal{G}_-$ reduces the form $\mathfrak{b}$ and let U be the direct rotation from the subspace $\mathcal{H}_+$ to the reducing subspace $\mathcal{G}_+$. Also assume that the decomposition $\mathcal{H} = \mathcal{G}_+ \oplus \mathcal{G}_-$ is $\mathcal{H}^1_A$-regular, where A is the diagonal self-adjoint operator given by* (2.4)*.*

Then

$$\widehat{\mathfrak{b}}[f, g] = \mathfrak{b}[Uf, Ug], \quad f, g \in \mathrm{Dom}[\widehat{\mathfrak{b}}] = \mathrm{Dom}[\mathfrak{b}],$$

is a diagonal form with respect to the decomposition $\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-$.

Proof. Due to Theorem 6.2, the Riccati equation (6.1) holds if and only if the decomposition $\mathcal{H} = \mathcal{G}_+ \oplus \mathcal{G}_-$ reduces the form. Then a straightforward computation shows that

$$\mathfrak{b}[(I+Y)f, h] = \mathfrak{a}[f, (I-Y)h] + \mathfrak{v}[Yf, (I-Y)h], \quad f, h \in \mathrm{Dom}[\mathfrak{a}].$$

Then, taking $h = (I-Y)^{-1}g$ with $g \in \mathrm{Dom}[\mathfrak{a}]$, one obtains that

$$\mathfrak{b}[(I+Y)f, (I-Y)^{-1}g] = \mathfrak{a}[f, g] + \mathfrak{v}[Yf, g], \quad f, g \in \mathrm{Dom}[\mathfrak{a}]. \tag{6.5}$$

Since the form $\mathfrak{a}$ is diagonal, and both the form $\mathfrak{v}$ and the operator Y are off-diagonal, it follows that the form $\mathfrak{d}[f, g] = \mathfrak{b}[(I+Y)f, (I-Y)^{-1}g]$ on $\mathrm{Dom}[\mathfrak{d}] = \mathrm{Dom}[\mathfrak{a}]$, is a diagonal form.

Since $U = (I+Y)|I+Y|^{-1} = (I-Y)^{-1}|I-Y|$ and $|I-Y| = |I+Y|$ is a diagonal operator, the equation (6.5) yields

$$\mathfrak{b}[Uf, Ug] = \mathfrak{a}[|I+Y|^{-1}f, |I-Y|g] + \mathfrak{v}[Y|I+Y|^{-1}f, |I-Y|g], \quad f, g \in \mathrm{Dom}[\mathfrak{a}],$$

provided that $|I+Y| = (I-Y^2)^{1/2}$ is bijective on $\mathrm{Dom}[\mathfrak{a}]$, which, in turn, follows along similar lines as in the proof of Lemma 4.2. □

It should be noted that the proof of Theorem 6.5, compared to the one of Theorem 5.1 (i), neither requires the domain stability condition to hold nor the semi-definiteness of the corresponding reducing graph subspaces $\mathcal{G}_\pm$. If, however, the domain stability condition holds, the proof of Theorem 5.1 (i) shows that the diagonalization procedure for the unbounded form $\mathfrak{b}$ in $\mathcal{H}$ can be reduced to the one of the corresponding bounded self-adjoint operator $\mathcal{B}$ in the space $\mathcal{H}_A^1$ (see (5.2)). The form $\widehat{\mathfrak{b}}$ then splits into the sum of two diagonal forms $\pm\widehat{\mathfrak{b}}_\pm$,

$$\widehat{\mathfrak{b}} = \widehat{\mathfrak{b}}_+ \oplus (-\widehat{\mathfrak{b}}_-),$$

that are not necessarily semi-bounded. However, if the saddle point form $\mathfrak{b}$ is *a priori* semi-bounded, the domain stability condition holds automatically and the corresponding diagonal forms $\pm\widehat{\mathfrak{b}}_\pm$ are semi-bounded and closed. In other words, in this case the statement of Theorem 6.5 can naturally be extended to the format of the one in Theorem 5.1.

7. Some applications

In this section, having in mind applications of the developed formalism to the study of the block Stokes operator from fluid dynamics, cf. [10, 17, 20], we focus on the class of saddle point forms provided by Example 2.4 in the semi-bounded situation.

We start by the following compactness result that may be of independent interest.

Lemma 7.1. *Let $\mathfrak{b}$ be the saddle point form from Example 2.4 and B the associated operator. Assume that $A_+ > 0$ and that the operator A_- is bounded and has compact resolvent. Then the positive spectral subspace of the operator B is a graph subspace,*

$$\mathrm{Ran}\,(\mathsf{E}_B((0,\infty))) = \mathrm{Graph}(\mathcal{H}_+, X)$$

with $X\colon \mathcal{H}_+ \to \mathcal{H}_-$ a compact contraction.

If, in addition, A_+^{-1} is in the Schatten–von Neumann ideal $\mathfrak{S}_p$, then X belongs to $\mathfrak{S}_{2p}$.

Proof. By Theorem 3.3,

$$\mathrm{Ran}(\mathsf{E}_B((0,\infty))) \oplus (\mathrm{Ker}(B) \cap \mathcal{H}_+) = \mathcal{G}(\mathcal{H}_+, X),$$

with X a contraction.

By [37, Theorem 1.3], we have that

$$\mathrm{Ker}(B) = (\mathrm{Ker}(A_+) \cap \mathcal{K}_+) \oplus (\mathrm{Ker}(A_-) \cap \mathcal{K}_-),$$

where

$$\mathcal{K}_\pm = \big\{x_\pm \in \mathcal{H}_\pm \mid \mathfrak{v}[x_+, x_-] = 0 \text{ for all } x_\mp \in \mathrm{Dom}[\mathfrak{a}_\mp]\big\}.$$

Therefore, if $A_+ > 0$, then $\mathrm{Ker}(B) \cap \mathcal{H}_+ = \{0\}$, which proves that

$$\mathrm{Ran}(\mathsf{E}_B((0,\infty)) = \mathrm{Graph}(\mathcal{H}_+, X).$$

Since the reducing subspace $\mathrm{Ran}(\mathsf{E}_B(0,\infty))$ is a graph subspace, the form Riccati equation (6.1) holds. Notice that the Riccati equation (6.1) can also be rewritten as the following quadratic equation

$$\mathfrak{a}_+[-X^*y, x] - \mathfrak{a}_-[y, Xx] + \mathfrak{v}[-X^*y, Xx] + \mathfrak{v}[y, x] = 0, \qquad (7.1)$$
$$x \in \mathrm{Dom}[\mathfrak{a}_+] \subseteq \mathcal{H}_+, \quad y \in \mathrm{Dom}[\mathfrak{a}_-] \subseteq \mathcal{H}_-,$$

for a "weak solution" X.

First, we claim that

$$(I + A_+^{-1/2} X^* W A_+^{-1/2}) A_+^{1/2} X^* = ((W + A_- X) A_+^{-1/2})^*. \qquad (7.2)$$

Indeed, since

$$\mathfrak{a}_+[-X^*y, x] = -\langle A_+^{1/2} X^* y, A_+^{1/2} x\rangle,$$
$$\mathfrak{a}_-[y, Xx] = \langle y, A_- X x\rangle,$$

and

$$\mathfrak{v}[-X^*y, Xx] + \mathfrak{v}[y, x] = -\langle W X^* y, Xx\rangle + \langle y, Wx\rangle,$$
$$x \in \mathrm{Dom}[\mathfrak{a}_+], \quad y \in \mathrm{Dom}[\mathfrak{a}_-] = \mathcal{H}_-,$$

equation (7.1) can be rewritten as

$$\langle (A_+^{1/2} + A_+^{-1/2} X^* W) X^* y, A_+^{1/2} x\rangle = \langle ((W + A_- X) A_+^{-1/2})^* y, A_+^{1/2} x\rangle,$$
$$x \in \mathrm{Dom}[\mathfrak{a}_+], \quad y \in \mathrm{Dom}[\mathfrak{a}_-] = \mathcal{H}_-.$$

Taking into account that $A_+^{1/2}$ is a surjective map from $\mathrm{Dom}[\mathfrak{a}_+]$ onto $\mathcal{H}_+$, we have

$$(I + A_+^{-1/2} X^* W A_+^{-1/2}) A_+^{1/2} X^* = (A_+^{1/2} + A_+^{-1/2} X^* W) X^*.$$

Since $\mathrm{Dom}((A_+)^{1/2}) \subseteq \mathrm{Dom}(W)$ and W is a closable operator by hypothesis, the operator $W A_+^{-1/2}$ is bounded in $\mathcal{H}_+$ (see, e.g., [21, Problem 5.22]). In particular, $(W + A_- X) A_+^{-1/2}$ is bounded and the claim follows by taking into account that

$$(A_+^{1/2} + A_+^{-1/2} X^* W) X^* = ((W + A_- X) A_+^{-1/2})^*.$$

To complete the proof of the lemma, one observes that $A_+ + X^* W$ is similar to $\widehat{B}_+$ and since the kernel of B is trivial, the kernel of the operator $A_+ + X^* W$ is trivial as well. Hence, the kernel of the Fredholm operator

$$F = I + A_+^{-1/2} X^* W A_+^{-1/2}$$

is also trivial (here we used that the operator $W A_+^{-1/2}$ is bounded and that $A_+^{-1/2}$ is compact). Hence F has a bounded inverse and then, from (7.2), we get that

$$X^* = A_+^{-1/2} [F^{-1} ((W + A_- X) A_+^{-1/2})^*]. \qquad (7.3)$$

Since $A_+^{-1/2}$ is compact, it follows that X^* is compact, so is X. From this representation it also follows that $A_+^{-1/2}$ and X share the same Schatten class membership. □

Remark 7.2. Note that in the situation of Lemma 7.1, in the particular case where the off-diagonal part W of the operator matrix (2.9) is a bounded operator, from (7.3) it also follows (see, e.g., [42, Satz 3.23]) that X belongs to the same Schatten–von Neumann ideal $\mathfrak{S}_p$ as A_+^{-1} does, cf. [40, Corollary 2.9.2].

As an illustration consider the following example.

Example 7.3 (The Stokes operator revisited). Assume that Ω is a bounded C^2-domain in $\mathbb{R}^d$, $d \geq 2$. In the direct sum of Hilbert spaces

$$\mathcal{H} = \mathcal{H}_+ \oplus \mathcal{H}_-,$$

where $\mathcal{H}_+ = L^2(\Omega)^d$ is the "velocity space" and $\mathcal{H}_- = L^2(\Omega)$ the "pressure space", introduce the block Stokes operator S via the symmetric sesquilinear form

$$\begin{aligned}\mathfrak{s}[v \oplus p, u \oplus q] &= \nu\langle \mathbf{grad}\ v, \mathbf{grad}\ u\rangle - v_*\langle \operatorname{div} v, q\rangle - v_*\langle p, \operatorname{div} u\rangle \qquad (7.4)\\ &=: \mathfrak{a}_+[v, u] + \mathfrak{v}[v \oplus p, u \oplus q],\end{aligned}$$

$$\operatorname{Dom}[\mathfrak{s}] = \{v \oplus p \,|\, v \in H_0^1(\Omega)^d,\ p \in L^2(\Omega)\}.$$

Here **grad** denotes the component-wise application of the standard gradient operator defined on the Sobolev space $H_0^1(\Omega)$, with $\nu > 0$ and $v_* \geq 0$ parameters.

It is easy to see that the Stokes operator S defined as the self-adjoint operator associated with the saddle point form $\mathfrak{s}$, is the Friedrichs extension of the operator matrix

$$\dot{S} = \begin{pmatrix} -\nu\mathbf{\Delta} & v_* \operatorname{grad} \\ -v_* \operatorname{div} & 0 \end{pmatrix}_{\mathcal{H}_+\oplus\mathcal{H}_-} \qquad (7.5)$$

defined on

$$\operatorname{Dom}(\dot{S}) = ((H^2(\Omega) \cap H_0^1(\Omega))^d \oplus H_0^1(\Omega).$$

Here $\mathbf{\Delta} = \Delta \cdot I_d$ is the vector-valued Dirichlet Laplacian, with I_d the identity operator in $\mathbb{C}^d$, div is the maximal divergence operator from $\mathcal{H}_+$ to $\mathcal{H}_-$ on

$$\operatorname{Dom}(\operatorname{div}) = \{v \in L^2(\Omega)^d \mid \operatorname{div} v \in L^2(\Omega)\},$$

and $(-\operatorname{grad})$ is its adjoint.

It is also known that the closure of the operator matrix

$$\mathbf{S} = \begin{pmatrix} -\nu\mathbf{\Delta} & v_* \operatorname{grad} \\ -v_* \operatorname{div} & 0 \end{pmatrix}_{\mathcal{H}_+\oplus\mathcal{H}_-}$$

naturally defined on a slightly different domain

$$\operatorname{Dom}(\mathbf{S}) = (H^2(\Omega) \cap H_0^1(\Omega))^d \oplus H^1(\Omega) \supset \operatorname{Dom}(\dot{S})$$

is self-adjoint (see [10]), which yields another characterization for the operator $S = S(\nu, v_*)$.

Clearly the set $C_0^\infty(\Omega)^d \oplus C_0^\infty(\Omega)$ is a core for the form $\mathfrak{s}$ and the operator S, so the form $\mathfrak{s}$ and the Friedrichs extension of the operator matrices $\dot{S}$ or $\mathbf{S}$ define the same operator.

We also remark that the Stokes operator is not an off-diagonal operator perturbation of the diagonal (unperturbed) operator $S(\nu,0)$ defined on

$$\mathrm{Dom}(S(\nu,0)) = (H^2(\Omega) \cap H_0^1(\Omega))^d \oplus L^2(\Omega)$$

for the operator matrix (7.5) is not a closed operator.

The following proposition can be considered a natural addendum to the known results for the Stokes operator [4, 10, 17, 20, 29, 33], see also [40, Example 2.4.11].

Proposition 7.4. *Let $\lambda_1(\Omega)$ be the first eigenvalue of the Dirichlet Laplacian on the bounded domain $\Omega \subset \mathbb{R}^d$, $d \geq 2$. Then*

(i) *The positive spectral subspace of the Stokes operator S can be represented as the graph of a contractive operator $X\colon L^2(\Omega)^d \to L^2(\Omega)$ with*

$$\|X\| \leq \tan\left(\frac{1}{2}\arctan \mathrm{Re}^*\right) < 1, \tag{7.6}$$

where

$$\mathrm{Re}^* = \frac{2v_*}{\nu\sqrt{\lambda_1(\Omega)}}; \tag{7.7}$$

(ii) *The operator X belongs to the Schatten–von Neumann ideal $\mathfrak{S}_p$ for any $p > d$;*

(iii) *The corresponding direct rotation U from the "velocity subspace" $L^2(\Omega)^d$ to the positive spectral subspace of the Stokes operator S maps the domain of the form onto itself. That is,*

$$U\big(H_0^1(\Omega)^d \oplus L^2(\Omega)\big) = H_0^1(\Omega)^d \oplus L^2(\Omega). \tag{7.8}$$

In particular, the form (7.4) and the Stokes operator S can be block diagonalized by the unitary transformation U.

Proof. (i). Due to the embedding

$$\mathrm{Dom}((-\boldsymbol{\Delta})^{1/2}) = H_0^1(\Omega)^d \subset \{v \in L^2(\Omega)^d \mid \operatorname{div} v \in L^2(\Omega)\} = \mathrm{Dom}(\operatorname{div}),$$

the entries of the operator matrix $\dot{S}$ satisfy the hypothesis of Example 2.4, so that the sesquilinear form $\mathfrak{s}$ is a saddle point form by Lemma 2.5. The first part of the assertion (i) then follows from Lemma 7.1.

To complete the proof of (i) it remains to check the estimate (7.6).

Recall that if P and Q are orthogonal projections and $\mathrm{Ran}(Q)$ is the graph of a bounded operator X from $\mathrm{Ran}(P)$ to $\mathrm{Ran}(P^\perp)$, then the operator angle Θ between the subspaces $\mathrm{Ran}(P)$ and $\mathrm{Ran}(Q)$ is a unique self-adjoint operator in the Hilbert space $\mathcal{H}$ with the spectrum in $[0,\pi/2]$ such that

$$\sin^2\Theta = PQ^\perp|_{\mathrm{Ran}(P)}.$$

In this case,

$$\|X\| = \tan\|\Theta\| \tag{7.9}$$

(see, e.g., [22, Eq. (3.12)]).

Using the estimate [20]

$$\tan 2\,\|\Theta\| \leq \frac{2v_*}{\nu\sqrt{\lambda_1((\Omega)}}$$

for the operator angle Θ between the "velocity subspace" $\mathcal{H}_+ = L^2(\Omega)^d$ and the positive spectral subspace $\mathcal{L}_+ = \mathrm{Ran}(\mathsf{E}_S((0,\infty))$ of the Stokes operator, one gets the bound (7.6) as a consequence of (7.9).

(ii). Denote by $\lambda_k(\Omega)$ the k^{th}-eigenvalue counting multiplicity of the Dirichlet Laplacian on the domain $\Omega \subset \mathbb{R}^d$, $d \geq 2$. By the Weyl's law, the following asymptotics

$$\lambda_k(\Omega) \sim \frac{4\pi^2 k^{2/d}}{(|B_d||\Omega|)^{2/d}} \quad (\text{as} \quad k \to \infty)$$

holds, see, e.g., [5, Theorem 5.1] (here $|B_d|$ is the volume of the unit ball in $\mathbb{R}^d$ and $|\Omega|$ is the volume of the domain Ω). Hence, the resolvent of the vector-valued Dirichlet Laplacian $\boldsymbol{\Delta}$ belongs to the ideal $\mathfrak{S}_p$ for any $p > d/2$. Then, by Lemma 7.1, we have that

$$X \in \mathfrak{S}_p, \quad \text{for any} \quad p > d,$$

which completes the proof of (ii).

(iii). Since $\mathfrak{s}$ is a semi-bounded saddle point form, one can apply Theorem 5.1 to justify (7.8) as well as the remaining statements of the proposition. □

Remark 7.5. The first part of the assertion (i) is known. It can be verified, for instance, by combing Theorem 2.7.7, Remark 2.7.12 and Proposition 2.7.13 in [40].

The generalized Reynolds number $\mathrm{Re}^* = \frac{2v_*}{\nu\sqrt{\lambda_1(\Omega)}}$ given by (7.7) has been introduced by Ladyzhenskaya in connection with her analysis of stability of solutions of the $2D$-Navier–Stokes equations in bounded domains [27]. To the best of our knowledge, the estimate (7.6), the Schatten class membership $X \in \mathfrak{S}_p$, $p > d$, as well as the mapping property (7.8) of the direct rotation U are new. We also note that the diagonalization of S by a similarity transformation has already been discussed and the one by a unitary operator has been indicated, see [40, Theorem 2.8.1].

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Solutions of Gross–Pitaevskii Equation with Periodic Potential in Dimension Two

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Dedicated to the Memory of Boris Pavlov

Abstract. Quasi-periodic solutions of a nonlinear polyharmonic equation for the case $4l > n+1$ in $\mathbb{R}^n$, $n > 1$, are studied. This includes Gross–Pitaevskii equation in dimension two ($l = 1, n = 2$). It is proven that there is an extensive "non-resonant" set $\mathcal{G} \subset \mathbb{R}^n$ such that for every $\vec{k} \in \mathcal{G}$ there is a solution asymptotically close to a plane wave $Ae^{i\langle \vec{k}, \vec{x}\rangle}$ as $|\vec{k}| \to \infty$, given A is sufficiently small.

1. Introduction

Let us consider a nonlinear polyharmonic equation with a periodic potential $V(\vec{x})$ and quasi-periodic boundary condition:

$$(-\Delta)^l u(\vec{x}) + V(\vec{x})u(\vec{x}) + \sigma|u(\vec{x})|^2 u(\vec{x}) = \lambda u(\vec{x}), \quad \vec{x} \in [0, 2\pi]^n, \tag{1}$$

$$\begin{cases} u(x_1, \ldots, \underbrace{2\pi}_{s\text{-th}}, \ldots, x_n) = e^{2\pi i t_s} u(x_1, \ldots, \underbrace{0}_{s\text{-th}}, \ldots, x_n), \\ \frac{\partial}{\partial x_s} u(x_1, \ldots, \underbrace{2\pi}_{s\text{-th}}, \ldots, x_n) = e^{2\pi i t_s} \frac{\partial}{\partial x_s} u(x_1, \ldots, \underbrace{0}_{s\text{-th}}, \ldots, x_n), \\ \vdots \\ \frac{\partial^{2l-1}}{\partial x_s^{2l-1}} u(x_1, \ldots, \underbrace{2\pi}_{s\text{-th}}, \ldots, x_n) = e^{2\pi i t_s} \frac{\partial^{2l-1}}{\partial x_s^{2l-1}} u(x_1, \ldots, \underbrace{0}_{s\text{-th}}, \ldots, x_n), \\ s = 1, \ldots, n. \end{cases} \tag{2}$$

where l is an integer, $4l > n + 1$, $\vec{t} = (t_1, \ldots, t_n) \in K = [0, 1]^n$, σ is a real number, $V(\vec{x})$ is a trigonometric polynomial, and

$$\int_Q V(\vec{x})d\vec{x} = 0,$$

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with $Q = [0, 2\pi]^n$ being the elementary cell of period 2π. More precisely,

$$V(\vec{x}\,) = \sum_{q \neq 0, |q| \leq R_0} v_q e^{i\langle q, \vec{x} \rangle}, \tag{3}$$

v_q being Fourier coefficients.

When $l = 1$, $n = 1, 2, 3$, equation (1) is a famous Gross–Pitaevskii equation for Bose–Einstein condensate, see, e.g., [5]. In physics papers, e.g., [3, 4, 6, 7], a big variety of numerical computations for Gross–Pitaevskii equation is made. However, they are restricted to the one dimensional case and there is a lack of theoretical considerations even for the case $n = 1$. In this paper we study the case $4l > n + 1$ which includes $l = 1, n = 2$.

The goal of this paper is to construct asymptotic formulas for $u(\vec{x}\,)$ as $\lambda \to \infty$. We show that there is an extensive "non-resonant" set $\mathcal{G} \subset \mathbb{R}^n$ such that for every $\vec{k} \in \mathcal{G}$ there is a quasi-periodic solution of (1) close to a plane wave $Ae^{i\langle \vec{k}, \vec{x} \rangle}$ with $\lambda = \lambda(\vec{k}, A)$ close to $\left|\vec{k}\right|^{2l} + \sigma|A|^2$ as $\left|\vec{k}\right| \to \infty$ (Theorem 3.11). We assume $A \in \mathbb{C}$ and $|A|$ is sufficiently small:

$$|\sigma||A|^2 < \lambda^\gamma, \quad \gamma < 2l - n. \tag{4}$$

Note that γ is any negative number for the Gross–Pitaevskii equation $l = 1, n = 2$. The quasi-momentum $\vec{t}$ in (1) is defined by the formula: $\vec{k} = \vec{t} + 2\pi j$, $j \in \mathbb{Z}^n$.

We show that the non-resonant set $\mathcal{G}$ has an asymptotically full measure in $\mathbb{R}^n$:

$$\lim_{R \to \infty} \frac{|\mathcal{G} \cap B_R|_n}{|B_R|_n} = 1, \tag{5}$$

where B_R is a ball of radius R in $\mathbb{R}^n$ and $|\cdot|_n$ is Lebesgue measure in $\mathbb{R}^n$.

Moreover, we investigate a set $\mathcal{D}(\lambda, A)$ of vectors $\vec{k} \in \mathcal{G}$, corresponding to a fixed sufficiently large λ and a fixed A. The set $\mathcal{D}(\lambda, A)$, defined as a level (isoenergetic) set for $\lambda(\vec{k}, A)$,

$$\mathcal{D}(\lambda, A) = \left\{ \vec{k} \in \mathcal{G} : \lambda(\vec{k}, A) = \lambda \right\}, \tag{6}$$

is proven to be a slightly distorted n-dimensional sphere with a finite number of holes (Theorem 3.13). For any sufficiently large λ, it can be described by the formula:

$$\mathcal{D}(\lambda, A) = \left\{ \vec{k} : \vec{k} = \varkappa(\lambda, A, \vec{\nu})\vec{\nu},\ \vec{\nu} \in \mathcal{B}(\lambda) \right\}, \tag{7}$$

where $\mathcal{B}(\lambda)$ is a subset of the unit sphere S_{n-1}. The set $\mathcal{B}(\lambda)$ can be interpreted as a set of possible directions of propagation for almost plane waves. Set $\mathcal{B}(\lambda)$ has an asymptotically full measure on S_{n-1} as $\lambda \to \infty$:

$$|\mathcal{B}(\lambda)| =_{\lambda \to \infty} \omega_{n-1} + O\left(\lambda^{-\delta}\right), \quad \delta > 0, \tag{8}$$

here $|\cdot|$ is the standard surface measure on S_{n-1}, $\omega_{n-1} = |S_{n-1}|$. The value $\varkappa(\lambda, A, \vec{\nu})$ in (7) is the "radius" of $\mathcal{D}(\lambda, A)$ in a direction $\vec{\nu}$. The function

$$\varkappa(\lambda, A, \vec{\nu}) - \left(\lambda - \sigma|A|^2\right)^{1/2l}$$

describes the deviation of $\mathcal{D}(\lambda, A)$ from the perfect sphere (circle) of the radius $(\lambda - \sigma|A|^2)^{1/2l}$ in $\mathbb{R}^n$. It is proven that the deviation is asymptotically small:

$$\varkappa(\lambda, A, \vec{\nu}) =_{\lambda\to\infty} \left(\lambda - \sigma|A|^2\right)^{1/2l} + O\left(\lambda^{-\gamma_1}\right), \quad \gamma_1 > 0. \tag{9}$$

To prove the results above, we consider the term $V+\sigma|u|^2$ in equation (1) as a periodic potential and formally change the nonlinear equation to a linear equation with an unknown potential $V(\vec{x}\,) + \sigma|u(\vec{x}\,)|^2$:

$$(-\Delta)^l u(\vec{x}\,) + \big(V(\vec{x}\,) + \sigma|u(\vec{x}\,)|^2\big)u(\vec{x}\,) = \lambda u(\vec{x}\,).$$

Further, we use known results for linear polyharmonic equations with periodic potentials. To start with, we consider a linear operator in $L^2(Q)$ described by the formula:

$$H(\vec{t}\,) = (-\Delta)^l + V, \tag{10}$$

and quasi-periodic boundary condition (2). The free operator $H_0(\vec{t}\,)$, corresponding to $V = 0$, has eigenfunctions given by:

$$\psi_j(\vec{x}\,) = e^{i\langle\vec{p}_j(\vec{t}\,),\vec{x}\rangle}, \quad \vec{p}_j(\vec{t}\,) := \vec{t} + 2\pi j, \quad j \in \mathbb{Z}^n,\ \vec{t} \in K, \tag{11}$$

and the corresponding eigenvalues $p_j^{2l}(\vec{t}\,) := \left|\vec{p}_j(\vec{t}\,)\right|^{2l}$. Perturbation theory for a linear operator $H(\vec{t}\,)$ with a periodic potential V is developed in [1]. It is shown that at high energies, there is an extensive set of generalized eigenfunctions being close to plane waves. Below (see Theorem 2.2) we describe this result in details. Now, we define a map $\mathcal{M} : L^\infty(Q) \to L^\infty(Q)$ by the formula:

$$\mathcal{M}W(\vec{x}\,) = V(\vec{x}\,) + \sigma\left|u_{\widetilde{W}}(\vec{x}\,)\right|^2. \tag{12}$$

Here, $\widetilde{W}$ is a shift of W by a constant such that $\int_Q \widetilde{W}(\vec{x}\,)d\vec{x} = 0$,

$$\widetilde{W}(\vec{x}\,) = W(\vec{x}\,) - \frac{1}{(2\pi)^n}\int_Q W(\vec{x}\,)d\vec{x}, \tag{13}$$

and $u_{\widetilde{W}}$ is an eigenfunction of the linear operator $(-\Delta)^l + \widetilde{W}$ with the boundary condition (2). Next, we consider a sequence $\{W_m\}_{m=0}^\infty$:

$$W_0 = V + \sigma|A|^2, \quad \mathcal{M}W_m = W_{m+1}. \tag{14}$$

Note that the sequence is well-defined by induction, since for each $m = 1, 2, 3, \ldots$ and $\vec{t}$ in a non-resonant set $\mathcal{G}$ described in Sect. 2, there is an eigenfunction $u_m(\vec{x}\,)$ corresponding to the potential $\widetilde{W}_m$:

$$H_m(\vec{t}\,)u_m = \lambda_m u_m,$$
$$H_m(\vec{t}\,)u_m := (-\Delta)^l u_m + \widetilde{W}_m u_m,$$

with λ_m, u_m being defined by formal series of the form (22)–(25), (33) with $\widetilde{W}_m$ instead of V. Those series are proven to be convergent, thus justifying our construction. Next, we prove that the sequence $\{W_m\}_{m=0}^\infty$ is a Cauchy sequence of periodic functions in Q with respect to a norm

$$\|W\|_* = \sum_{q\in\mathbb{Z}^n} |w_q|, \tag{15}$$

w_q being Fourier coefficients of W. This implies that

$$W_m \to W \text{ with respect to the norm } \|\cdot\|_*, \ W \text{ is a periodic function.}$$

Further, we show that

$$u_m \to u_{\widetilde{W}} \text{ in } L^\infty(Q), \qquad \lambda_m \to \lambda_{\widetilde{W}} \text{ in } \mathbb{R},$$

where $u_{\widetilde{W}}$, $\lambda_{\widetilde{W}}$ correspond to the potential $\widetilde{W}$ (via (22)–(25), (33) with $\widetilde{W}$ instead of V). It follows from (12) and (14) that $\mathcal{M}W = W$ and, hence, $u := u_{\widetilde{W}}$ solves the nonlinear equation (1) with quasi-periodic boundary condition (2).

Note that the results of the paper can be easily generalized for the case of a sufficiently smooth potential $V(x)$. Generalization for the case $l = 1, n = 3$ (Gross–Pitaevskii equation in dimension three) is also possible. However, it requires more subtle considerations than here and will be done in a forthcoming paper.

The paper is organized as follows. In Sect. 2, we introduce results for the linear operator $(-\Delta)^l + V$ which include the perturbation formulas for an eigenvalue and its spectral projection. In Sect. 3, we prove existence of solutions of the equation (1) with boundary condition (2) and investigate their properties. Isoenergetic surfaces are also introduced and described there.

2. Linear Operator

Let us consider an operator

$$H = (-\Delta)^l + V, \tag{16}$$

in $L^2(\mathbb{R}^n)$, $4l > n+1$ and $n \geq 2$ where l is an integer and $V(\vec{x})$ is defined by (3). Since $V(\vec{x})$ is periodic with an elementary cell Q, the spectral study of (16) can be reduced to that of a family of Bloch operators $H(\vec{t}\,)$ in $L^2(Q)$, $\vec{t} \in K$ (see formula (10) and quasi-periodic conditions (2)).

The free operator $H_0(\vec{t}\,)$, corresponding to $V = 0$, has eigenfunctions given by (11) and the corresponding eigenvalue is $p_j^{2l}(\vec{t}\,) := |\vec{p}_j(\vec{t}\,)|^{2l}$. Next, we describe an isoenergetic surface of $H_0(\vec{t}\,)$ in K. To start with, we consider the sphere $S(k)$ of radius k centered at the origin in $\mathbb{R}^n$. For each $j \in \mathbb{Z}^n$ such that $(j+K)\cap S(k) \neq \emptyset$, $K := [0,1]^n$, we translate the corresponding piece of $S(k)$ into K, thus obtaining the sphere of radius k "packed" into K. We denote it by $S_0(k)$. Namely,

$$S_0(k) = \left\{\vec{t} \in K : \text{ there is a } \ j \in \mathbb{Z}^n \text{ such that } p_j^{2l}(\vec{t}\,) = k^{2l}\right\}.$$

Obviously, operator $H_0(\vec{t}\,)$ has an eigenvalue equal to k^{2l} if and only if $\vec{t} \in S_0(k)$. For this reason, $S_0(k)$ is called an isoenergetic surface of $H_0(\vec{t}\,)$. When $\vec{t}$ is a point of self-intersection of $S_0(k)$, there exists $q \neq j$ such that

$$p_q^{2l}(\vec{t}\,) = p_j^{2l}(\vec{t}\,). \tag{17}$$

In other words, there is a non-simple eigenvalue of $H_0(\vec{t}\,)$. We remove from the set $S_0(k)$ the $(k^{-n+1-\delta})$-neighborhoods of all self-intersections (17). We call the remaining set a non-resonant set and denote is by $\chi_0(k,\delta)$, The removed neighborhood of self-intersections is relatively small and, therefore, $\chi_0(k,\delta)$ has asymptotically full measure with respect to $S_0(k)$:

$$\frac{|\chi_0(k,\delta)|}{|S_0(k)|} = 1 + O\big(k^{-\delta/8}\big),$$

here and below $|\cdot|$ is Lebesgue measure of a surface in $\mathbb{R}^n$. It can be easily shown that for any $\vec{t} \in \chi_0(k,\delta)$, there is a unique $j \in \mathbb{Z}^n$ such that $p_j^{2l}(\vec{t}\,) = k^{2l}$ and

$$\min_{q\neq j} \big|p_q^{2l}(\vec{t}\,) - p_j^{2l}(\vec{t}\,)\big| > k^{2l-n-\delta}. \tag{18}$$

This means that the distance from $p_j^{2l}(\vec{t}\,)$ to the nearest eigenvalue $p_q^{2l}(\vec{t}\,)$, $q \neq j$ is greater than $k^{2l-n-\delta}$. If $2l > n$, then this distance is large and standard perturbation series can be constructed for $p_j^{2l}(\vec{t}\,)$, $t \in \chi_0(k,\delta)$. However, the denseness of the eigenvalues increases infinitely when $k \to \infty$ and $2l < n$. Hence, eigenvalues of the free operator $H_0(\vec{t}\,)$ strongly interact with each other when $2l < n$, the case $2l = n$ being intermediate. Nevertheless, the perturbation series for eigenvalues and their spectral projections were constructed in [1] for $4l > n+1$ when $\vec{t}$ belongs to a non-resonant set χ_1.

Lemma 2.1. *For any* $0 < \beta < (4l-n-1)/(n-1)$, $0 < 2\delta < 4l-n-1-\beta(n-1)$ *and sufficiently large* $k > k_0(\beta,\delta)$, *there is a non-resonant set* $\chi_1(k,\beta,\delta)$ *such that for any* $t \in \chi_1(k,\beta,\delta)$ *there is a unique* $j \in \mathbb{Z}^n$: $p_j^{2l}(\vec{t}\,) = k^{2l}$ *and if* $\vec{t}$ *is in the* $(k^{-n+1-2\delta})$*-neighborhood of* $\chi_1(k,\beta,\delta)$ *in* K, *then for* $z \in C_0 = \big\{z \in \mathbb{C} : |z - k^{2l}| = k^{2l-n-\delta}\big\}$ *we have*

$$\min_{i\in\mathbb{Z}^n} \big|p_i^{2l}(\vec{t}\,) - z\big| > k^{2l-n-\delta}, \tag{19}$$

$$200\big|p_i^{2l}(\vec{t}\,) - z\big|\big|p_{i+q}^{2l}(\vec{t}\,) - z\big| > k^{2\gamma_2}, \quad i \in \mathbb{Z}^n,\ |q| < k^\beta,\ q \neq 0, \tag{20}$$

here and below:

$$2\gamma_2 = 4l - n - 1 - \beta(n-1) - 2\delta > 0. \tag{21}$$

The non-resonant set $\chi_1(k,\beta,\delta)$ *has an asymptotically full measure on* $S_0(k)$*:*

$$\frac{s\big(S_0(k) \setminus \chi_1(k,\beta,\delta)\big)}{s\big(S_0(k)\big)} = O\big(k^{-\delta/8}\big).$$

Theorem 2.2. *Under the conditions of Lemma* 2.1, *there exists a single eigenvalue of the operator* $H(\vec{t}\,)$ *in the interval* $\varepsilon(k,\delta) \equiv \big(k^{2l} - k^{2l-n-\delta}, k^{2l} + k^{2l-n-\delta}\big)$. *It is given by the series*

$$\lambda(\vec{t}\,) = p_j^{2l}(\vec{t}\,) + \sum_{r=2}^{\infty} g_r(k,t), \tag{22}$$

converging absolutely, where the index j is uniquely determined from the relation $p_j^{2l}(\vec{t}\,) \in \varepsilon(k,\delta)$ and

$$g_r(k,\vec{t}\,) = \frac{(-1)^r}{2\pi i r} \operatorname{Tr} \oint_{C_0} \Big(\big(H_0(\vec{t}\,) - z\big)^{-1} V \Big)^r dz. \tag{23}$$

The spectral projection, corresponding to $\lambda(\vec{t}\,)$ is given by the series

$$E(t) = E_j + \sum_{r=1}^{\infty} G_r(k,t), \tag{24}$$

which converges in the trace class S_1 uniformly, where

$$G_r(k,\vec{t}\,) = \frac{(-1)^{r+1}}{2\pi i} \oint_{C_0} \Big(\big(H_0(\vec{t}\,) - z\big)^{-1} V \Big)^r \big(H_0(\vec{t}\,) - z\big)^{-1} dz. \tag{25}$$

Moreover, for coefficients $g_r(k,\vec{t}\,), G_r(k,\vec{t}\,)$, the following estimates hold:

$$|g_r(k,\vec{t}\,)| < k^{2l-n-\delta} k^{-\gamma_2 r}, \tag{26}$$

$$\|G_r(k,\vec{t}\,)\|_{S_1} \le \hat{v} k^{-\gamma_2 r}, \quad \hat{v} = cR_0^n \max_{m \in \mathbb{Z}^n} |v_m|. \tag{27}$$

Remark 2.3. We use the following norm $\|T\|_1$ of an operator T in $l_2(\mathbb{Z}^2)$:

$$\|T\|_1 = \max_i \sum_p |T_{pi}|.$$

It can be easily seen from construction in [1] that estimates (27) hold with respect to this norm, too.

Let us introduce the notations:

$$T(m) \equiv \frac{\partial^{|m|}}{\partial t_1^{m_1} \partial t_2^{m_2} \cdots \partial t_n^{m_n}}, \tag{28}$$

$$|m| \equiv m_1 + m_2 + \cdots + m_n, \quad m! \equiv m_1! m_2! \cdots m_n!,$$

$$0 \le |m| < \infty, \quad T(0)f \equiv f.$$

The following theorem and corollary are proven in [1].

Theorem 2.4. *Under the conditions of Theorem 2.2, the series* (22), (24) *can be differentiated with respect to $\vec{t}$ any number of times, and they retain their asymptotic character. Coefficients $g_r(k,\vec{t}\,)$ and $G_r(k,\vec{t}\,)$ satisfy the following estimates in the $(k^{-n+1-2\delta})$-neighborhood in $\mathbb{C}^n$ of the nonsingular set $\chi_1(k,\beta,\delta)$:*

$$\big|T(m) g_r(k,\vec{t}\,)\big| < m!\, k^{2l-n-\delta} (\hat{v} k^{-\gamma_2})^r k^{|m|(n-1+2\delta)}, \tag{29}$$

$$\big\|T(m) G_r(k,\vec{t}\,)\big\|_1 < m! (\hat{v} k^{-\gamma_2})^r k^{|m|(n-1+2\delta)}. \tag{30}$$

Corollary 2.5. *There are the estimates for the perturbed eigenvalue and its spectral projection:*

$$\big|T(m)\big(\lambda(\vec{t}\,) - p_j^{2l}(\vec{t}\,)\big)\big| < c\, m!\, k^{(n-1+2\delta)|m|} k^{2l-n-\delta-2\gamma_2}, \tag{31}$$

$$\big\|T(m)\big(E(\vec{t}\,) - E_j\big)\big\|_1 < c\, m!\, k^{(n-1+2\delta)|m|} k^{-\gamma_2}. \tag{32}$$

Corollary 2.6. *There is a one-dimensional space of Bloch eigenfunctions u_0 corresponding to the projection $E(t)$ given by* (24)*. They are given by the formula:*

$$u_0(\vec{x}\,) = AE\big(\vec{t}\,\big)e^{i\langle \vec{p}_j(\vec{t}\,),\vec{x}\rangle} = A\sum_{m\in\mathbb{Z}^n} E\big(\vec{t}\,\big)_{mj}e^{i\langle \vec{p}_m(\vec{t}\,),\vec{x}\rangle}$$
$$= Ae^{i\langle \vec{p}_j(\vec{t}\,),\vec{x}\rangle}\left(1+\sum_{q\neq 0}\frac{v_q}{p_j^{2l}\big(\vec{t}\,\big)-p_{j+q}^{2l}\big(\vec{t}\,\big)}e^{i\langle \vec{p}_q(\vec{0}),\vec{x}\rangle}+\cdots\right),$$

for $j,q\in\mathbb{Z}^n$, $A\in\mathbb{C}$.

Let $\widetilde{\chi}_1(k,\beta,\delta)\subset S(k)$ be the image of $\chi_1(k,\beta,\delta)\subset S_0(k)$ on the sphere $S(k)$:

$$\widetilde{\chi}_1(k,\beta,\delta) = \big\{\vec{p}_j\big(\vec{t}\,\big)\in S(k):\ \vec{t}\in\chi_1(k,\beta,\delta)\big\}. \tag{33}$$

Note that $\widetilde{\chi}_1(k,\beta,\delta)$ is well-defined, since $\chi_1(k,\beta,\delta)$ does not contain self intersections of $S_0(k)$. Let $\mathcal{B}(\lambda)\subset S_{n-1}$ be the set of directions corresponding to the nonsingular set $\widetilde{\chi}_1(k,\beta,\delta)$:

$$\mathcal{B}(\lambda) = \big\{\vec{\nu}\in S_{n-1}: k\vec{\nu}\in\widetilde{\chi}_1(k,\beta,\delta)\big\},\quad k^{2l}=\lambda. \tag{34}$$

The set $\mathcal{B}(\lambda)$ can be interpreted as a set of possible directions of propagation for almost plane waves (33). We define the non-resonance set $\mathcal{G}\subset\mathbb{R}^n$ as the union of all $\widetilde{\chi}_1(k,\beta,\delta)$:

$$\mathcal{G} = \bigcup_{k>k_0(\beta,\delta)}\widetilde{\chi}_1(k,\beta,\delta) \tag{35}$$

Further we denote vectors of $\mathcal{G}$ by $\vec{k}$. Formulas (34), (35) yield

$$\mathcal{G} = \big\{\vec{k}=k\vec{\nu}:\vec{\nu}\in\mathcal{B}\big(k^{2l}\big),\ k>k_0(\beta,\delta)\big\}. \tag{36}$$

Since any vector $\vec{k}$ can be written as $\vec{k}=\vec{p}_j(t)$ in a unique way, formula (35) yields:

$$\mathcal{G} = \big\{\vec{p}_j\big(\vec{t}\,\big):\ \vec{t}\in\chi_1(k,\beta,\delta),\ \text{where } k=p_j\big(\vec{t}\,\big),\ k>k_0(\beta,\delta)\big\}. \tag{37}$$

Let $\lambda(\vec{k})$ be defined by (22), where $\vec{k}=\vec{p}_j\big(\vec{t}\,\big)$.

Next, we describe isoenergetic surfaces for the operator (16). The set $\mathcal{D}(\lambda)$, defined as a level (isoenergetic) set for $\lambda(\vec{k})$,

$$\mathcal{D}(\lambda) = \left\{\vec{k}\in\mathcal{G}:\lambda(\vec{k})=\lambda\right\}. \tag{38}$$

Lemma 2.7. *For any sufficiently large λ, $\lambda>k_0(\beta,\delta)^{2l}$, and for every $\vec{\nu}\in\mathcal{B}(\lambda)$, there is a unique $\varkappa=\varkappa(\lambda,\vec{\nu})$ in the interval*

$$I:=\big[k-k^{-n+1-2\delta},k+k^{-n+1-2\delta}\big],\quad k^{2l}=\lambda,$$

such that

$$\lambda(\varkappa\vec{\nu})=\lambda. \tag{39}$$

Furthermore, $|\varkappa-k|\leq ck^{2l-n-\delta-2\gamma_2-2l+1}=ck^{-\gamma_1}$, $\gamma_1=4l-2-\beta(n-1)-\delta>0$.

The lemma easily follows from (31) for $|m|=1$.

Lemma 2.8. 1. *For any sufficiently large λ, $\lambda > k_0(\beta,\delta)^{2l}$, the set $\mathcal{D}(\lambda)$, defined by* (38) *is a distorted sphere with holes; it is described by the formula:*

$$\mathcal{D}(\lambda) = \left\{\vec{k} : \vec{k} = \varkappa(\lambda,\vec{\nu})\vec{\nu},\ \vec{\nu} \in \mathcal{B}(\lambda)\right\}, \tag{40}$$

where $\varkappa(\lambda,\vec{\nu}) = k + h(\lambda,\vec{\nu})$ and $h(\lambda,\vec{\nu})$ obeys the inequalities:

$$|h| < ck^{-\gamma_1}, \quad |\nabla_{\vec{\nu}} h| < ck^{-\gamma_1+n-1+2\delta} = ck^{-2\gamma_2+\delta}. \tag{41}$$

2. *The measure of $\mathcal{B}(\lambda) \subset S_{n-1}$ satisfies the estimate* (8).
3. *The surface $\mathcal{D}(\lambda)$ has the measure that is asymptotically close to that of the whole sphere of the radius k in the sense that*

$$\left|\mathcal{D}(\lambda)\right| \underset{\lambda\to\infty}{=} \omega_{n-1}k^{n-1}\left(1 + O(k^{-\delta})\right), \quad \lambda = k^{2l}. \tag{42}$$

The proof is based on Implicit Function Theorem.

3. Proof of The Main Result

First, we prove that $\{W_m\}_{m=0}^{\infty}$ in (14) is a Cauchy sequence with respect to the norm defined by (15). Further we need the following obvious properties of norm $\|\cdot\|_*$:

$$\|f\|_* = \|\overline{f}\|_*, \quad \|\Re(f)\|_* \le \|f\|_*, \quad \|\Im(f)\|_* \le \|f\|_*, \quad \|fg\|_* \le \|f\|_*\|g\|_*. \tag{43}$$

where $\Re(f)$ and $\Im(f)$ are real and imaginary part for f, respectively.

We define the value $k_1 = k_1(\|V\|_*,\delta,\beta)$ as

$$k_1(\|V\|_*,\delta,\beta) = \max\left\{ (16\|V\|_*)^{1/\gamma_2},\ k_0(\beta,\delta)\right\}, \tag{44}$$

with $\gamma_2 > 0$ being defined by (21) and $k_0(\beta,\delta)$ as in Corollary 2.1.

Lemma 3.1. *The following inequalities hold for any $m = 1,2,\ldots$:*

$$\|\widetilde{W}_m - V\|_* \le 8|\sigma||A|^2\|V\|_* k^{-\gamma_2}, \tag{45}$$

$$\|W_m - W_{m-1}\|_* \le 4|\sigma||A|^2\|V\|_* k^{-\gamma_2}(|\sigma||A|^2k^{-\gamma_0})^{m-1}, \tag{46}$$

$$\|E_m(\vec{t}\,) - E_{m-1}(\vec{t}\,)\|_1 \le 8|\sigma||A|^2\|V\|_* k^{-(2l-n-\delta)-\gamma_2}(|\sigma||A|^2k^{-\gamma_0})^{m-1}, \tag{47}$$

where $\gamma_0 = 2l - n - 2\delta$, $\delta > 0$, and $|\sigma||A|^2 < k^{\gamma_0-\delta}$, k being sufficiently large $k > k_1(\|V\|_*,\delta,\beta)$.

Corollary 3.2. *There is a periodic function W such that W_m converges to W with respect to the norm $\|\cdot\|_*$:*

$$\|W - W_m\|_* \le 8|\sigma||A|^2\|V\|_* k^{-\gamma_2}(|\sigma||A|^2k^{-\gamma_0})^{m}. \tag{48}$$

Proof of Lemma 3.1. Let us consider the function (33) written in the form

$$u_0(\vec{x}\,) = \psi_0(\vec{x}\,)e^{i\langle \vec{p}_j(\vec{t}\,),\vec{x}\rangle}, \tag{49}$$

where

$$\psi_0(\vec{x}\,) = A \sum_{q\in\mathbb{Z}^n} E\big(\vec{t}\,\big)_{j+q,j} e^{i\langle \vec{p}_q(\vec{0}),\vec{x}\rangle}, \tag{50}$$

is called the periodic part of u_0.

First, we prove (46) for $m = 1$. It follows from (12), (14) and (43) that

$$\begin{aligned}\big\|W_1 - W_0\big\|_* &= |\sigma|\big\||u_0|^2 - |A|^2\big\|_* = |\sigma|\big\||\psi_0|^2 - |A|^2\big\|_* \\ &\le |\sigma|\big\||\psi_0|^2 - |A|^2 + 2i\Im(\bar{A}\psi_0)\big\|_* = |\sigma|\big\|(\psi_0 - A)(\overline{\psi}_0 + \bar{A})\big\|_* \\ &\le |\sigma|\big\|\psi_0 - A\big\|_*\big\|\overline{\psi}_0 + \bar{A}\big\|_*. \end{aligned} \tag{51}$$

Let us consider

$$B_0(z) = (H_0\big(\vec{t}\,\big) - z)^{-\frac{1}{2}} V (H_0\big(\vec{t}\,\big) - z)^{-\frac{1}{2}}. \tag{52}$$

Then it follows from Lemma 2.1 that

$$\max_{z\in C_0} \Big\|(H_0\big(\vec{t}\,\big) - z)^{-1}\Big\|_1 < k^{-2l+n+\delta}, \tag{53}$$

$$\max_{z\in C_0} \|B_0(z)\|_1 < \|V\|_* k^{-\gamma_2}, \tag{54}$$

with γ_2 being defined by (21). By (25) and (52),

$$G_r(k,\vec{t}\,) = \frac{(-1)^{r+1}}{2\pi i} \oint_{C_0} \big(H_0\big(\vec{t}\,\big) - z\big)^{-\frac{1}{2}} B_0(z)^r \big(H_0\big(\vec{t}\,\big) - z\big)^{-\frac{1}{2}} dz. \tag{55}$$

It is easy to see that

$$\big\|G_r(k,\vec{t}\,)\big\|_1 < \|V\|_*^r k^{-\gamma_2 r}. \tag{56}$$

Next, by (50), (25) and (27),

$$\begin{aligned}\|\psi_0 - A\|_* &\le \Big|AE\big(\vec{t}\,\big)_{jj} - A\Big| + |A| \sum_{q\in\mathbb{Z}^n\setminus\{0\}} \Big|E\big(\vec{t}\,\big)_{j+q,j}\Big| \\ &\le |A| \sum_{r=1}^{\infty} \|G_r(k,\vec{t}\,)\|_1 \le \|V\|_*|A|k^{-\gamma_2}(1 + o(1)). \end{aligned} \tag{57}$$

It follows that

$$\|\psi_0\|_* = \|\overline{\psi}_0\|_* \le |A| + O\big(|A|k^{-\gamma_2}\big). \tag{58}$$

Using (51), (57) and (58), we get

$$\|W_1 - W_0\|_* \le 4|\sigma||A|^2\|V\|_* k^{-\gamma_2}.$$

Since $\|\widetilde{W}_1 - V\|_* = \|\widetilde{W}_1 - \widetilde{W}_0\|_* \le \|W_1 - W_0\|_*$, we have

$$\|\widetilde{W}_1 - V\|_* \le 4|\sigma||A|^2\|V\|_* k^{-\gamma_2}. \tag{59}$$

Now, we use mathematical induction to show simultaneously:

$$\big\|\widetilde{W}_m - V\big\|_* \le 8|\sigma||A|^2\|V\|_* k^{-\gamma_2}, \tag{60}$$

$$\|W_m - W_{m-1}\|_* \le 4|\sigma||A|^2\|V\|_* k^{-\gamma_2}\big(|\sigma||A|^2 k^{-\gamma_0}\big)^{m-1}. \tag{61}$$

Suppose that for all $1 \le s \le m-1$,

$$\|\widetilde{W}_s - V\|_* \le 8|\sigma||A|^2\|V\|_* k^{-\gamma_2}, \tag{62}$$

$$\|W_s - W_{s-1}\|_* \le 4|\sigma||A|^2\|V\|_* k^{-\gamma_2}(|\sigma||A|^2 k^{-\gamma_0})^{s-1}. \tag{63}$$

Let, by analogy with (33),

$$u_s(\vec{x}\,) := A \sum_{m\in\mathbb{Z}^n} E_s\big(\vec{t}\,\big)_{m,j} e^{i\langle \vec{p}_m(\vec{t}\,),\vec{x}\rangle}, \tag{64}$$

where $E_s\big(\vec{t}\,\big)$ is the spectral projection (24) with the potential $\widetilde{W}_s$. Obviously,

$$u_s(\vec{x}\,) = \psi_s(\vec{x}\,)e^{i\langle \vec{p}_j(\vec{t}\,),\vec{x}\rangle}, \tag{65}$$

where the function

$$\psi_s(\vec{x}\,) = A \sum_{q\in\mathbb{Z}^n} E_s\big(\vec{t}\,\big)_{j+q,j} e^{i\langle \vec{p}_q(\vec{0}\,),\vec{x}\rangle} \tag{66}$$

is the periodic part of u_s. Clearly,

$$\|\psi_s\|_* \le |A|\big\|E_s\big(\vec{t}\,\big)\big\|_1. \tag{67}$$

Let

$$B_s(z) = \big(H_0\big(\vec{t}\,\big) - z\big)^{-\frac{1}{2}}\widetilde{W}_s\big(H_0\big(\vec{t}\,\big) - z\big)^{-\frac{1}{2}}. \tag{68}$$

Using (62), (54) and (19), we easily obtain

$$\|B_s(z)\|_1 \le 8|\sigma||A|^2\|V\|_* k^{-2l+n+\delta-\gamma_2} + \|V\|_* k^{-\gamma_2} \le 2\|V\|_* k^{-\gamma_2}, \quad z \in C_0, \tag{69}$$

for any $1 \le s \le m-1$. It is easy to see now that

$$\|G_{s,r}(k,\vec{t}\,)\|_1 \le \big(4\|V\|_* k^{-\gamma_2}\big)^r, \quad 1 \le s \le m-1, \tag{70}$$

here $G_{s,r}(k,\vec{t}\,)$ is given by (25) with $\widetilde{W}_s$ instead of V. It follows that

$$\begin{aligned} \|E_s\big(\vec{t}\,\big)\|_1 &\le 1 + \sum_{r=1}^{\infty} \big\|G_{s,r}\big(k,\vec{t}\,\big)\big\|_1 \\ &\le 1 + 8\|V\|_* k^{-\gamma_2} \le 2, \quad 1 \le s \le m-1. \end{aligned} \tag{71}$$

Next, we note that

$$\begin{aligned} &\max_{z\in C_0} \|B^r_{m-1}(z) - B^r_{m-2}(z)\|_1 \\ &\le \max_{z\in C_0} \|B_{m-1}(z) - B_{m-2}(z)\|_1 \left(\|B_{m-1}(z)\|_1 + \|B_{m-2}(z)\|_1\right)^{r-1} \\ &\le k^{-(2l-n-\delta)}\big\|\widetilde{W}_{m-1} - \widetilde{W}_{m-2}\big\|_*\Big(4\|V\|_* k^{-\gamma_2}\Big)^{r-1}. \end{aligned} \tag{72}$$

Hence,

$$\begin{aligned} &\|G_{m-1,r}(k,\vec{t}\,) - G_{m-2,r}(k,\vec{t}\,)\|_1 \\ &\quad \le k^{-(2l-n-\delta)}\big\|\widetilde{W}_{m-1} - \widetilde{W}_{m-2}\big\|_*\Big(4\|V\|_* k^{-\gamma_2}\Big)^{r-1}. \end{aligned} \tag{73}$$

Estimate (73) yields

$$\big\|E_{m-1}(\vec t\,)-E_{m-2}(\vec t\,)\big\|_1 \le \sum_{r=1}^{\infty}\big\|G_{m-1,r}(k,\vec t\,)-G_{m-2,r}(k,\vec t\,)\big\|_1 \le 2k^{-(2l-n-\delta)}\big\|\widetilde W_{m-1}-\widetilde W_{m-2}\big\|_*. \tag{74}$$

Next, considering as in (51), we obtain:

$$\big\|W_m-W_{m-1}\big\|_* \le |\sigma|\big\|\psi_{m-1}-\psi_{m-2}\big\|_*\big\|\overline{\psi}_{m-1}+\overline{\psi}_{m-2}\big\|_*, \tag{75}$$

and, hence, by (66),

$$\|W_m-W_{m-1}\|_* \le |\sigma||A|^2\big\|E_{m-1}(\vec t\,)-E_{m-2}(\vec t\,)\big\|_1\left(\|E_{m-1}(\vec t\,)\|_1+\big\|E_{m-2}(\vec t\,)\big\|_1\right). \tag{76}$$

Using (71) and (74), we obtain

$$\|W_m-W_{m-1}\|_* \le 8|\sigma||A|^2k^{-(2l-n-\delta)}\|\widetilde W_{m-1}-\widetilde W_{m-2}\|_*. \tag{77}$$

Considering $\big\|\widetilde W_{m-1}-\widetilde W_{m-2}\big\|_* \le \|W_{m-1}-W_{m-2}\|_*$ and using (63) for $s=m-1$, we arrive at the estimate:

$$\begin{aligned}\|W_m-W_{m-1}\|_* &\le 8|\sigma||A|^2k^{-(2l-n-\delta)}4|\sigma||A|^2\|V\|_*k^{-\gamma_2}\left(|\sigma||A|^2k^{-\gamma_0}\right)^{m-2} \\ &\le 4|\sigma||A|^2\|V\|_*k^{-\gamma_2}\left(|\sigma||A|^2k^{-\gamma_0}\right)^{m-1},\end{aligned} \tag{78}$$

when $k>k_1(\|V\|_*,\delta,\beta)$. Further, (78) and (59) enable the estimate

$$\begin{aligned}\big\|\widetilde W_m-V\big\|_* &\le \big\|\widetilde W_m-\widetilde W_{m-1}\big\|_*+\big\|\widetilde W_{m-1}-\widetilde W_{m-2}\big\|_*+\cdots+\big\|\widetilde W_1-V\big\|_* \\ &\le 8|\sigma||A|^2\|V\|_*k^{-\gamma_2},\end{aligned}$$

which completes the proof of (45) and (46). Using (74), we obtain (47). □

Lemma 3.3. *Suppose $\vec t$ belongs to the $(k^{-n+1-2\delta})$-neighborhood in K of the non-resonant set $\chi_1(k,\beta,\delta)$. Then for every sufficiently large $k>k_1(\|V\|_*,\delta,\beta)$ and every $A\in\mathbb{C}:|\sigma||A|^2<k^{\gamma_0-\delta}$, the sequence $E_m(\vec t\,)$ converges with respect to $\|\cdot\|_1$ to a one-dimensional spectral projection $E_{\widetilde W}(\vec t\,)$ of $H_0(t)+\widetilde W$:*

$$\big\|E_m(\vec t\,)-E_{\widetilde W}(\vec t\,)\big\|_1 \le 8\|V\|_*k^{-\gamma_2}\left(|\sigma||A|^2k^{-\gamma_0}\right)^{m+1}. \tag{79}$$

The projection $E_{\widetilde W}(\vec t\,)$ is given by the series (24), (25) *with $\widetilde W$ instead of V. The series converges with respect to $\|\cdot\|_1$:*

$$\big\|G_r(k,\vec t\,)\big\|_1 \le \left(2\|V\|_*k^{-\gamma_2}\right)^r \tag{80}$$

Proof. Let $B(z)$ be given by (68) with $\widetilde W$ instead of $\widetilde W_s$. Obviously, $B(z)$ is the limit of $B_m(z)$ in $\|\cdot\|_1$-norm. The estimate (69) yields:

$$\|B(z)\|_1 \le 2\|V\|_*k^{-\gamma_2},\quad z\in C_0. \tag{81}$$

It follows that the perturbation series for the resolvent of $H_0(\vec t\,)+W$ converges with respect to $\|\cdot\|_1$ norm on C_0. Integrating the series of z we obtain that $E(t)$

admits the expansion (24), (25) and (80) holds. Obviously, G_r corresponding to $\widetilde{W}$ is the limit of $G_{m,r}$ in $\|\cdot\|_1$ norm. Summing the estimates (74), we obtain (79). □

Definition 3.4. Let $u(\vec{x})$ be defined as in Corollary 2.6 for the potential $\widetilde{W}(\vec{x})$. Let $\psi(\vec{x})$ be the periodic part of $u(\vec{x})$.

The next lemma follows from the estimate (79).

Lemma 3.5. *Suppose $\vec{t}$ belongs to the $(k^{-n+1-2\delta})$-neighborhood in K of the non-resonant set $\chi_1(k,\beta,\delta)$. Then for every sufficiently large $k > k_1(\|V\|_*,\delta,\beta)$ and every $A \in \mathbb{C} : |\sigma||A|^2 < k^{\gamma_0-\delta}$, the sequence $\psi_m(\vec{x})$ converges to the function $\psi(\vec{x})$ with respect to $\|\cdot\|_*$:*

$$\|\psi_m - \psi\|_* \leq 8|A|\|V\|_* k^{-\gamma_2}(|\sigma||A|^2 k^{-\gamma_0})^{m+1}. \tag{82}$$

Corollary 3.6. *The sequence u_m converges to u in $L^\infty(Q)$.*

Corollary 3.7.

$$\mathcal{M}W = W.$$

Proof of Corollary 3.7. Considering as in (75), we obtain:

$$\big\|\mathcal{M}W_m - \mathcal{M}W\big\|_* \leq |\sigma|\big\|\psi_m - \psi\big\|_*\big\|\overline{\psi}_m + \overline{\psi}\big\|_*, \tag{83}$$

It immediately follows from Lemma 3.3 that $\mathcal{M}W_m \to \mathcal{M}W$ with respect to $\|\cdot\|_*$. Now, by (14) and (83), we have $\mathcal{M}W = W$. □

Let $\lambda_m(\vec{t}\,)$, $\lambda_{\widetilde{W}}(\vec{t}\,)$ be the eigenvalues (22) corresponding to $\widetilde{W}_m$ and $\widetilde{W}$, respectively.

Lemma 3.8. *Under conditions of Lemma* 3.3 *the sequence $\lambda_m(\vec{t}\,)$ converges to $\lambda_{\widetilde{W}}(\vec{t}\,)$ being given by* (22) *and*

$$|g_r(k,\vec{t}\,)| < r^{-1}k^{2l-n-\delta}\left(4\|V\|_* k^{-\gamma_2}\right)^r, \tag{84}$$

where g_r is given by (23) *with $\widetilde{W}$ instead of V.*

Proof. By perturbation theory, $\lambda_{\widetilde{W}}(\vec{t}\,)$ is the limit of $\lambda_m(\vec{t}\,)$ as $m \to \infty$. Let us show that the series (22) converges. Let us consider two projections $E_0 = E_j$, $E_1 = I - E_j$, here E_j is the spectral projection of H_0, see (25). Note that

$$\oint_{C_0} (E_1 B(z) E_1)^r \, dz = 0, \quad r = 1, 2, \dots,$$

since the integrand is holomorphic inside C_0. Hence,

$$\begin{aligned}\oint_{C_0} B(z)^r dz &= \oint_{C_0} \left(B(z)^r - (E_1 B(z) E_1)^r\right) dz \\ &= \sum_{i_1,\dots,i_{r+1}=0,1,\exists s: i_s=0} \oint_{C_0} E_{i_1} B(z) E_{i_2} B(z) \cdots E_{i_r} B(z) E_{i_{r+1}} dz.\end{aligned}$$

Obviously, $E_{i_1}B(z)_{i_2}B(z)\cdots E_{i_r}B(z)E_{i_{r+1}}$ is in the trace class S_1 if at least one index i_s, $1 \le s \le r+1$ is zero, since $E_0 \in S_1$. Notice that for the adjoint operator B^* we have $B^*(z) = B(\bar{z})$. It follows:

$$\|E_{i_1}B(z)E_{i_2}B(z)\cdots E_{i_r}B(z)E_{i_{r+1}}\|_{S_1} \le \|B\|^r \le \|B^*\|_1^{r/2}\|B\|_1^{r/2} < \left(2\|V\|_* k^{-\gamma_2}\right)^r.$$

Now, we easily obtain (84). □

Considering as in the proof of Theorem 2.4, one can prove an analogous theorem:

Theorem 3.9. *Under the conditions of Lemma* 3.3 *the series* (22), (24) *for the potential $\widetilde{W}$ can be differentiated with respect to $\vec{t}$ any number of times, and they retain their asymptotic character. Coefficients $g_r(k,\vec{t}\,)$ and $G_r(k,\vec{t}\,)$ satisfy the following estimates in the $(k^{-n+1-2\delta})$-neighborhood in $\mathbb{C}^n$ of the nonsingular set $\chi_1(k,\beta,\delta)$:*

$$\left|T(m)g_r(k,\vec{t}\,)\right| < m!k^{2l-n-\delta}\left(4\|V\|_* k^{-\gamma_2}\right)^r k^{|m|(n-1+2\delta)}, \tag{85}$$

$$\left\|T(m)G_r(k,\vec{t}\,)\right\|_1 < m!(2\|V\|_* k^{-\gamma_2})^r k^{|m|(n-1+2\delta)}. \tag{86}$$

Corollary 3.10. *There are the estimates for the perturbed eigenvalue and its spectral projection:*

$$\left|T(m)\big(\lambda_{\widetilde{W}}(\vec{t}\,) - p_j^{2l}(\vec{t}\,)\big)\right| < C(\|V\|_*)m!k^{(n-1+2\delta)|m|}k^{2l-n-\delta-2\gamma_2}, \tag{87}$$

$$\left\|T(m)\big(E_{\widetilde{W}}(\vec{t}\,) - E_j\big)\right\|_1 < C(\|V\|_*)m!k^{(n-1+2\delta)|m|}k^{-\gamma_2}. \tag{88}$$

In particular,

$$\left|\lambda_{\widetilde{W}}(\vec{t}\,) - p_j^{2l}(\vec{t}\,)\right| < C(\|V\|_*)k^{2l-n-\delta-2\gamma_2}, \tag{89}$$

$$\left\|E_{\widetilde{W}}(\vec{t}\,) - E_j\right\|_1 < C(\|V\|_*)k^{-\gamma_2}, \tag{90}$$

$$\left|\nabla\lambda_{\widetilde{W}}(\vec{t}\,) - 2l\vec{p}_j(\vec{t}\,)p_j^{2l-2}(\vec{t}\,)\right| < C(\|V\|_*)k^{2l-1-2\gamma_2+\delta}. \tag{91}$$

We have the following main result for the nonlinear polyharmonic equation with quasi-periodic condition.

Theorem 3.11. *Suppose $\vec{t}$ belongs to the $(k^{-n+1-2\delta})$-neighborhood in K of the non-resonant set $\chi_1(k,\beta,\delta)$, $k > k_1(\|V\|_*,\delta,\beta)$ and $A \in \mathbb{C} : |\sigma||A|^2 < k^{\gamma_0-\delta}$. Then, there is a function $u(\vec{x}\,)$, depending on $\vec{t}$ as a parameter, and a real value $\lambda(\vec{t}\,)$, satisfying the equation*

$$(-\Delta)^l u(\vec{x}\,) + V(\vec{x}\,)u(\vec{x}\,) + \sigma|u(\vec{x}\,)|^2u(\vec{x}\,) = \lambda u(\vec{x}\,), \quad \vec{x} \in Q, \tag{92}$$

and the quasi-periodic boundary condition (2)*. The following formulas hold:*

$$u(\vec{x}\,) = Ae^{i\langle\vec{p}_j(\vec{t}\,),\vec{x}\rangle}\left(1 + \widetilde{u}(\vec{x}\,)\right), \tag{93}$$

$$\lambda(\vec{t}\,) = p_j^{2l}(\vec{t}\,) + \sigma|A|^2 + O\left(\left(k^{2l-n-\delta} + \sigma|A|^2\right)k^{-2\gamma_2}\right), \tag{94}$$

where $\widetilde{u}(\vec{x}\,)$ *is periodic and*

$$\|\widetilde{u}\|_* \leq k^{-\gamma_2}, \quad \gamma_2 > 0 \ \ \textit{is defined by } (21). \tag{95}$$

Proof. Let us consider the function u given by Definition 3.4 and the value $\lambda_{\widetilde{W}}(\vec{t}\,)$. They solve the equation

$$(-\Delta)^l u(\vec{x}\,) + \widetilde{W}(\vec{x}\,)u(\vec{x}\,) = \lambda_{\widetilde{W}}(\vec{t}\,)u(\vec{x}\,), \quad \vec{x} \in Q, \tag{96}$$

and u satisfies the quasi-boundary condition (2). By Corollary 3.7, we have

$$W(\vec{x}\,) = \mathcal{M}W(\vec{x}\,) = V(\vec{x}\,) + \sigma|u(\vec{x}\,)|^2.$$

Hence,

$$\widetilde{W}(\vec{x}\,) = W(\vec{x}\,) - \frac{1}{(2\pi)^n}\int_Q W(\vec{x}\,)d\vec{x} = V(\vec{x}\,) + \sigma|u(\vec{x}\,)|^2 - \sigma\|u\|^2_{L^2(Q)}.$$

Substituting the last expression into (96), we obtain that $u(\vec{x}\,)$ satisfies (92) with

$$\begin{aligned}\lambda(\vec{t}\,) &= \lambda_{\widetilde{W}}(\vec{t}\,) + \sigma\|u\|^2_{L^2(Q)} \\ &= \lambda_{\widetilde{W}}(\vec{t}\,) + \sigma|A|^2 \sum_{q\in Z^n} \left|\left(E_{\widetilde{W}}\right)_{qj}\right|^2 \\ &= \lambda_{\widetilde{W}}(\vec{t}\,) + \sigma|A|^2\left(E_{\widetilde{W}}\right)_{jj}.\end{aligned} \tag{97}$$

Note that $(G_1)_{jj} = 0$ and, therefore, $\left(E_{\widetilde{W}}\right)_{jj} = 1 + O(k^{-2\gamma_2})$. Further, by the definition of $u(\vec{x}\,)$, we have

$$u(\vec{x}\,) := Ae^{i\langle\vec{p}_j(\vec{t}\,),\vec{x}\rangle}\sum_{q\in\mathbb{Z}^n}\left(E_{\widetilde{W}}\right)_{q+j,j} e^{i\langle p_q(0),\vec{x}\rangle}. \tag{98}$$

Using formulas (97) and (98) and estimates (89) and (90), we obtain (93) and (95), respectively. □

Lemma 3.12. *For any sufficiently large* λ*, every* $A \in \mathbb{C} : |\sigma||A|^2 < k^{\gamma_0-\delta}$, $\lambda = k^{2l}$ *and for every* $\vec{\nu} \in \mathcal{B}(\lambda)$*, there is a unique* $\varkappa = \varkappa(\lambda, A, \vec{\nu})$ *in the interval*

$$I := \left[k - k^{-n+1-2\delta}, k + k^{-n+1+2\delta}\right],$$

such that

$$\lambda(\varkappa\vec{\nu}, A) = \lambda. \tag{99}$$

Furthermore,

$$\begin{aligned}|\varkappa(\lambda, A, \vec{\nu}) - \widetilde{k}| &\leq C(||V||_*)\left(k^{2l-n-\delta} + |\sigma||A|^2\right)k^{-2l+1-2\gamma_2}, \\ \widetilde{k} &= (\lambda - \sigma|A|^2)^{1/2l}.\end{aligned} \tag{100}$$

Proof. Taking into account (34) and using formulas (87), (91) and Implicit Function Theorem, we prove the lemma. The proof is completely analogous to that for the linear case. □

Theorem 3.13. 1. *For any sufficiently large* λ *and every* $A \in \mathbb{C} : |\sigma||A|^2 < k^{\gamma_0-\delta}$, *the set* $\mathcal{D}(\lambda, A)$, *defined by* (6) *is a distorted sphere with holes; it can be described by the formula*

$$\mathcal{D}(\lambda, A) = \left\{\vec{k} : \vec{k} = \varkappa(\lambda, A, \vec{\nu})\vec{\nu},\ \vec{\nu} \in \mathcal{B}(\lambda)\right\}, \tag{101}$$

where $\varkappa(\lambda, A, \vec{\nu}) = \widetilde{k} + h(\lambda, A, \vec{\nu})$ *and* $h(\lambda, A, \vec{\nu})$ *obeys the inequalities*

$$|h| < C(||V||_*) \left(k^{2l-n-\delta} + |\sigma||A|^2\right) k^{-2l+1-2\gamma_2} < C(||V||_*)k^{-\gamma_1}, \tag{102}$$

with $\gamma_1 = n - 1 + \delta + 2\gamma_2 > n - 1$,

$$\left|\nabla_{\vec{\nu}} h\right| < C(||V||_*)k^{-\gamma_1+n-1+2\delta} = C(||V||_*)k^{-2\gamma_2+\delta}. \tag{103}$$

2. *The measure of* $\mathcal{B}(\lambda) \subset S_{n-1}$ *satisfies the estimate*

$$L\left(\mathcal{B}\right) = \omega_{n-1}\left(1 + O\left(k^{-\delta}\right)\right). \tag{104}$$

3. *The surface* $\mathcal{D}(\lambda, A)$ *has the measure that is asymptotically close to that of the whole sphere of the radius* k *in the sense that*

$$\left|\mathcal{D}(\lambda, A)\right| \underset{\lambda\to\infty}{=} \omega_{n-1}k^{n-1}\left(1 + O\left(k^{-\delta}\right)\right). \tag{105}$$

Proof. The proof is based on Implicit Function Theorem. It is completely analogous to Lemma 2.11 in [1]. □

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The Integral Transform of N.I. Akhiezer

Victor Katsnelson

This paper is dedicated to Boris Pavlov, a great man and outstanding mathematician.

Abstract. We study the integral transform which appeared in a different form in Akhiezer's textbook "Lectures on Integral Transforms".

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1. The Akhiezer Integral Transforms: a formal definition

In the present paper we consider the one-parametric family of pairs $\boldsymbol{\Phi}_\omega, \boldsymbol{\Psi}_\omega$ of linear integral operators. The parameter ω which enumerates the family can be an arbitrary positive number and is fixed in the course of our consideration. Formally the operators $\boldsymbol{\Phi}_\omega, \boldsymbol{\Psi}_\omega$ are defined as convolution operators according the formulas

$$(\boldsymbol{\Phi}_\omega \boldsymbol{x})(t) = \int\limits_{\mathbb{R}} \Phi_\omega(t-\tau)\boldsymbol{x}(\tau)d\tau, \quad t \in \mathbb{R}, \tag{1.1a}$$

$$(\boldsymbol{\Psi}_\omega \boldsymbol{x})(t) = \int\limits_{\mathbb{R}} \Psi_\omega(t-\tau)\boldsymbol{x}(\tau)d\tau, \quad t \in \mathbb{R}. \tag{1.1b}$$

In (1.1), $\boldsymbol{x}(\tau)$ is 2×1 vector-column,

$$\boldsymbol{x}(\tau) = \begin{bmatrix} x_1(\tau) \\ x_2(\tau) \end{bmatrix}, \tag{1.2}$$

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which entries $x_1(\tau), x_2(\tau)$ are measurable functions, and Φ_ω, Ψ_ω are 2×2 matrices,

$$\Phi_\omega(t) = \begin{bmatrix} C_\omega(t) & S_\omega(t) \\ S_\omega(t) & C_\omega(t) \end{bmatrix}, \tag{1.3a}$$

$$\Psi_\omega(t) = \begin{bmatrix} C_\omega(t) & -S_\omega(t) \\ -S_\omega(t) & C_\omega(t) \end{bmatrix}, \tag{1.3b}$$

where

$$C_\omega(t) = \frac{\omega}{\pi}\cdot\frac{1}{\cosh \omega t}, \quad S_\omega(t) = \frac{\omega}{\pi}\cdot\frac{1}{\sinh \omega t}. \tag{1.4}$$

Here and in what follows, sinh, cosh, tanh, sech are hyperbolic functions.
For $z \in \mathbb{C}$,

$$\sinh z = \frac{e^z - e^{-z}}{2}, \quad \cosh z = \frac{e^z + e^{-z}}{2}, \quad \tanh z = \frac{e^z - e^{-z}}{e^z + e^{-z}}, \quad \operatorname{sech} z = \frac{2}{e^z + e^{-z}}.$$

The operators $\mathbf{\Phi}_\omega$, $\mathbf{\Psi}_\omega$ are naturally decomposed into blocks:

$$\mathbf{\Phi}_\omega = \begin{bmatrix} \boldsymbol{C}_\omega & \boldsymbol{S}_\omega \\ \boldsymbol{S}_\omega & \boldsymbol{C}_\omega \end{bmatrix}, \quad \mathbf{\Psi}_\omega = \begin{bmatrix} \boldsymbol{C}_\omega & -\boldsymbol{S}_\omega \\ -\boldsymbol{S}_\omega & \boldsymbol{C}_\omega \end{bmatrix}, \tag{1.5}$$

where $\boldsymbol{C}_\omega$ and $\boldsymbol{S}_\omega$ are convolution operators:

$$(\boldsymbol{C}_\omega x)(t) = \int\limits_{\mathbb{R}} C_\omega(t-\tau)x(\tau)d\tau, \tag{1.6a}$$

$$(\boldsymbol{S}_\omega x)(t) = \int\limits_{\mathbb{R}} S_\omega(t-\tau)x(\tau)d\tau. \tag{1.6b}$$

In (1.6), x is a $\mathbb{C}$-valued function.

The function $C_\omega(\xi)$ is continuous and positive on $\mathbb{R}$. It decays exponentially as $|\xi| \to \infty$:

$$\frac{\omega}{\pi}e^{-\omega|\xi|} \leq C(\xi) < \frac{2\omega}{\pi}e^{-\omega|\xi|}, \quad \forall\, \xi \in \mathbb{R}. \tag{1.7}$$

Since

$$|\tau| - |t| \leq |t-\tau| \leq |\tau| + |t|,$$

the convolution kernel $C(t-\tau)$ admits the estimate

$$\frac{\omega}{\pi}e^{-\omega|t|}e^{-\omega|\tau|} \leq C(t-\tau) < \frac{2\omega}{\pi}e^{\omega|t|}e^{-\omega|\tau|}, \quad \forall\, t \in \mathbb{R},\ \forall\, \tau \in \mathbb{R}. \tag{1.8}$$

Definition 1.1. *The set* L^1_ω as the set of all complex valued functions $x(t)$ which are measurable, defined almost everywhere with respect to the Lebesgue measure on $\mathbb{R}$ and satisfy the condition

$$\int\limits_{\mathbb{R}} |x(\xi)|e^{-\omega|\xi|}d\xi < \infty. \tag{1.9}$$

The set $L^1_\omega \dotplus L^1_\omega$ is the set of all 2×1 columns $\boldsymbol{x}(t) = \begin{bmatrix} x_1(t) \\ x_2(t) \end{bmatrix}$ such that $x_1(t) \in L^1_\omega$ and $x_2(t) \in L^1_\omega$.

Lemma 1.2. *Let* $x(\tau)$ *be a* $\mathbb{C}$*-valued function which belongs to the space* L^1_ω*. Then the integral in the right hand side of* (1.6a) *exists*[1] *for every* $t \in \mathbb{R}$*.*

We define the function $(\boldsymbol{C}_\omega x)(t)$ *by means of the equality* (1.6a)*.*

Remark 1.3. For $x(\tau) \in L^1_\omega$, the function $(\boldsymbol{C}_\omega x)(t)$ is a continuous function well defined on the whole $\mathbb{R}$. Nevertheless the function $(\boldsymbol{C}_\omega x)(t)$ may not belong to the space L^1_ω. The operator $\boldsymbol{C}_\omega$ does not map the space L^1_ω into itself. (In other words, the operator $\boldsymbol{C}_\omega$ considered as an operator in L^1_ω is unbounded.)

The situation with the integral in the right hand side of (1.6b) is more complicated. The function $S_\omega(\xi)$ also decays exponentially as $|\xi| \to \infty$:

$$|S(\xi)| < \frac{2\omega}{\pi(1 - e^{-2\omega|\xi|})} e^{-\omega|\xi|}, \quad \forall\, \xi \in \mathbb{R}. \tag{1.10}$$

However the function S_ω has the singularity at the point $\xi = 0$:

$$S_\omega(\xi) = \frac{1}{\pi\xi} + r(\xi), \tag{1.11}$$

where $r(\xi)$ is a function which is continuous and bounded for $\xi \in \mathbb{R}$. Thus the convolution kernel $S_\omega(t-\tau)$ has a non-integrable singularity on the diagonal $t = \tau$:

$$\int\limits_{(t-\varepsilon, t+\varepsilon)} |S_\omega(t-\tau)| d\tau = \infty, \quad \forall\, t \in \mathbb{R}, \forall\, \varepsilon > 0.$$

Therefore the integral in the right hand side of (1.6b) may not exist as a Lebesgue integral. Given a function $x(\tau)$, the equality

$$\int\limits_{\mathbb{R}} |S_\omega(t-\tau)x(\tau)| d\tau = \infty \tag{1.12}$$

holds at every point $t \in \mathbb{R}$ which is a Lebesgue point of the function x and $x(t) \neq 0$. Nevertheless, under the condition (1.9) we can attach a meaning to the integral $\int\limits_{\mathbb{R}} S_\omega(t-\tau)x(\tau)d\tau$ for almost every $t \in \mathbb{R}$.

Lemma 1.4. *Let* $x(\tau)$ *be a* $\mathbb{C}$*-valued function which belongs to the space* L^1_ω*. Then* the principal value integral

$$\text{p.v.} \int\limits_{\mathbb{R}} S_\omega(t-\tau)x(\tau)d\tau \stackrel{\text{def}}{=} \lim_{\varepsilon \to +0} \int\limits_{\mathbb{R}\setminus(t-\varepsilon, t+\varepsilon)} S_\omega(t-\tau)x(\tau)d\tau \tag{1.13}$$

exists for almost every $t \in \mathbb{R}$*.*

We define the function $(\boldsymbol{S}_\omega x)(t)$ *by means of the equality* (1.6b)*, where the integral in the right hand side of* (1.6b) *is interpreted as a principal value integral.*

---

[1]That is, the value of this integral is a *finite* complex number for every $t \in \mathbb{R}$.

Under the condition (1.9), the integral $\int\limits_{\mathbb{R}\setminus(t-\varepsilon,t+\varepsilon)} S_\omega(t-\tau)x(\tau)d\tau$ exists as a Lebesgue integral for every $\varepsilon > 0$:

$$\int\limits_{\mathbb{R}\setminus(t-\varepsilon,t+\varepsilon)} |S_\omega(t-\tau)x(\tau)|d\tau < \infty, \quad \forall\, t \in \mathbb{R},\, \forall\, \varepsilon > 0.$$

This follows from the estimate (1.10). The assertion that the limit in (1.13) exists for almost every $t \in \mathbb{R}$ will be proved in Sect. 4 using the Hilbert transform theory.

Remark 1.5. Under the assumption (1.9), the function

$$y(t) = \text{p.v.} \int\limits_{\mathbb{R}} S_\omega(t-\tau)x(\tau)d\tau,$$

which is defined for almost every t, is not necessary locally summable. It may happen that $\int\limits_{[a,b]} |y(t)|dt = \infty$ for every finite interval $[a,b]$, $-\infty < a < b < \infty$.

Let us define the transforms $\mathbf{\Phi}_\omega$ and $\mathbf{\Psi}_\omega$ formally.

Definition 1.6. For $\boldsymbol{x}(\tau) = \begin{bmatrix} x_1(\tau) \\ x_2(\tau) \end{bmatrix} \in L^1_\omega \dotplus L^1_\omega$, we put

$$(\mathbf{\Phi}_\omega \boldsymbol{x})(t) = \boldsymbol{y}(t), \quad (\mathbf{\Psi}_\omega \boldsymbol{x})(t) = \boldsymbol{z}(t), \tag{1.14}$$

where $\boldsymbol{y}(t)$ and $\boldsymbol{z}(t)$ are 2×1 columns:

$$\boldsymbol{y}(t) = \begin{bmatrix} y_1(t) \\ y_2(t) \end{bmatrix}, \quad \boldsymbol{z}(t) = \begin{bmatrix} z_1(t) \\ z_2(t) \end{bmatrix}, \tag{1.15}$$

with the entries

$$y_1(t) = (\boldsymbol{C}_\omega x_1)(t) + (\boldsymbol{S}_\omega x_2)(t), \quad z_1(t) = \quad (\boldsymbol{C}_\omega x_1)(t) - (\boldsymbol{S}_\omega x_2)(t), \tag{1.16a}$$

$$y_2(t) = (\boldsymbol{S}_\omega x_1)(t) + (\boldsymbol{C}_\omega x_2)(t), \quad z_2(t) = -(\boldsymbol{S}_\omega x_1)(t) + (\boldsymbol{C}_\omega x_2)(t). \tag{1.16b}$$

The operators $\boldsymbol{C}_\omega$ and $\boldsymbol{S}_\omega$ are the same that appeared in Lemmas 1.2 and 1.4, respectively.

According to Lemmas 1.2 and 1.4, the values $\boldsymbol{y}(t)$ and $\boldsymbol{z}(t)$ are well defined for almost every $t \in \mathbb{R}$.

The integral transforms (1.1)–(1.3) are said to be *the Akhiezer integral transforms.*

In another form, these transforms appear in [1, Chap. 15]. (See Problems 3 and 4 in Chap. 15.) The matrix nature of the Akhiezer transforms was camouflaged there.

In what follows, we consider the Akhiezer transform in various functional spaces. We show that the operators $\mathbf{\Phi}_\omega$ and $\mathbf{\Psi}_\omega$ are mutually inverse in spaces of functions growing *slower* than $e^{\omega|t|}$.

2. The operators $\boldsymbol{C}_\omega$ and $\boldsymbol{S}_\omega$ in $\boldsymbol{L^2}$

The Fourier transform machinery is an adequate tool for study convolution operators.

1. Studying the operators $\boldsymbol{C}_\omega$ and $\boldsymbol{S}_\omega$ by means of the Fourier transform technique, we deal with the spaces L^1 and L^2. Both these spaces consist of measurable functions defined almost everywhere on the real axis $\mathbb{R}$ with respect to the Lebesgue measure. The spaces are equipped by the standard linear operations and the standard norms. If $u \in L^1$, then

$$\|u\|_{L^1} = \int_{\mathbb{R}} |u(t)|dt. \tag{2.1}$$

The space L^1 consists of all u such that $\|u\|_{L^1} < \infty$. If $u \in L^2$, then

$$\|u\|_{L^2} = \Big\{ \int_{\mathbb{R}} |u(\xi)|^2 d\xi \Big\}^{1/2}. \tag{2.2}$$

The space L^2 consists of all u such that $\|u\|_{L^2} < \infty$. This space is equipped by inner product $\langle \cdot\,, \cdot \rangle_{L^2}$. If $u' \in L^2$, $u'' \in L^2$, then

$$\langle u', u'' \rangle_{L^2} = \int_{\mathbb{R}} u'(t)\overline{u''(t)}dt. \tag{2.3}$$

2. The Fourier–Plancherel operator $\mathfrak{F}$:

$$\mathfrak{F}u = \hat{u} \tag{2.4}$$

where

$$\hat{u}(\lambda) = \int_{\mathbb{R}} u(t)e^{it\lambda}dt, \tag{2.5}$$

maps the space L^2 *on*to itself isometrically:

$$\|\hat{u}\|^2_{L^2} = 2\pi\, \|u\|^2_{L^2}, \quad \forall\, u \in L^2. \tag{2.6}$$

The inverse operator $\mathfrak{F}^{-1}$ is of the form

$$\mathfrak{F}^{-1}v = \check{v}, \tag{2.7}$$

where

$$\check{v}(t) = \frac{1}{2\pi} \int_{\mathbb{R}} v(\lambda)e^{-it\lambda}d\lambda. \tag{2.8}$$

Lemma 2.1. *Let $f \in L^2$ and $k \in L^1$. Then*

1. *The integral*

$$g(t) = \int_{\mathbb{R}} k(t-\tau)f(\tau)d\tau \tag{2.9}$$

exists as a Lebesgue integral (i.e., $\int_{\mathbb{R}} |k(t-\tau)g(\tau)|d\tau < \infty$) for almost every $t \in \mathbb{R}$.

2. *The function g belongs to L^2, and the inequality*

$$\|g\|_{L^2} \leq \|k\|_{L^1} \|f\|_{L^2} \tag{2.10}$$

holds.

3. *The Fourier–Plancherel transforms $\hat{f}$ and $\hat{g}$ are related by the equality*

$$\hat{g}(\lambda) = \hat{k}(\lambda) \cdot \hat{f}(\lambda), \quad \text{for a.e. } \lambda \in \mathbb{R}, \tag{2.11}$$

where

$$\hat{k}(\lambda) = \int\limits_{\mathbb{R}} k(t) e^{it\lambda} dt, \quad \forall \lambda \in \mathbb{R}. \tag{2.12}$$

This lemma can be found in [2, Theorem 65]. See also [3, Theorem 3.9.4].

3. Let us calculate the Fourier transforms of the functions C_ω and S_ω. The function C_ω belongs to L^1. So its Fourier transform

$$\widehat{C_\omega}(\lambda) = \int\limits_{\mathbb{R}} C_\omega(t) e^{it\lambda} dt \tag{2.13}$$

is well defined for every $\lambda \in \mathbb{R}$.

Lemma 2.2. *The Fourier transforms $\widehat{C_\omega}(\lambda)$ of the function $C_\omega(t)$ is:*

$$\widehat{C_\omega}(\lambda) = \operatorname{sech} \frac{\pi\lambda}{2\omega}, \quad \forall \lambda \in \mathbb{R}. \tag{2.14}$$

The formula (2.14) can be found in [2], where it appears as (7.1.6).

4. The function $S_\omega(t)$ does not belong to L^1. This function has non-integrable singularity at the point $t = 0$. Therefore the integral $\int\limits_{\mathbb{R}} S_\omega(t) e^{2\pi it\lambda} dt$ does not exist as a Lebesgue integral. However, $\int\limits_{\mathbb{R}\setminus(-\varepsilon,\varepsilon)} |S_\omega(t)| dt < \infty$, $\forall \varepsilon > 0$. So the integral

$$\widehat{S_{\omega,\varepsilon}}(\lambda) = \int\limits_{\mathbb{R}\setminus(-\varepsilon,\varepsilon)} S_\omega(t) e^{it\lambda} dt \tag{2.15}$$

exists as a Lebesgue integral for every $\varepsilon > 0$. We *define* the Fourier transform $\widehat{S_\omega}(\lambda)$ as a principle value integral:

$$\widehat{S_\omega}(\lambda) = \lim_{\varepsilon \to +0} \int\limits_{\mathbb{R}\setminus(-\epsilon,\epsilon)} S_\omega(t) e^{it\lambda} dt. \tag{2.16}$$

Lemma 2.3. *The limit in* (2.16) *exists for every $\lambda \in \mathbb{R}$. The Fourier transforms $\widehat{S_\omega}(\lambda)$ of the function $S_\omega(t)$ is:*

$$\widehat{S_\omega}(\lambda) = i \cdot \tanh \frac{\pi\lambda}{2\omega}, \quad \forall \lambda \in \mathbb{R}. \tag{2.17}$$

The difference

$$\varrho_\omega(\lambda, \varepsilon) = \widehat{S_\omega}(\lambda) - \widehat{S_{\omega,\varepsilon}}(\lambda), \quad \forall \lambda \in \mathbb{R}, \varepsilon > 0. \tag{2.18}$$

satisfies the conditions

$$\lim_{\varepsilon\to+0} \varrho_\omega(\lambda,\varepsilon)=0, \quad \forall\,\lambda\in\mathbb{R}, \tag{2.19}$$

and

$$\sup_{\substack{\lambda\in\mathbb{R},\\ 0<\varepsilon\le\frac{\pi}{4\omega}}} \left|\varrho_\omega(\lambda,\varepsilon)\right| < \infty. \tag{2.20}$$

The formula (2.17) can be found in [2], where it appears as (7.2.3).

5. In Sect. 1 we already have defined the functions $\boldsymbol{C}_\omega x$ and $\boldsymbol{S}_\omega x$ for x from the space L^1_ω. The space L^2 is contained in L^1_ω. If $x\in L^2$, then

$$\int\limits_{\mathbb{R}} |x(t)|e^{-\omega|t|}dt \le \Big\{\int\limits_{\mathbb{R}} |x(t)|^2dt\Big\}^{1/2}\Big\{\int\limits_{\mathbb{R}} e^{-2\omega|t|}dt\Big\}^{1/2} < \infty. \tag{2.21}$$

According to Lemmas 1.2 and 1.4, if $f\in L^1_\omega$, then the function $(\boldsymbol{C}_\omega f)(t)$ is defined for every $t\in\mathbb{R}$ and the function $(\boldsymbol{S}_\omega f)(t)$ is defined for almost every $t\in\mathbb{R}$. However, for $f\in L^2(\mathbb{R})$, we can obtain much more accurate results.

Lemma 2.4. *Let $f\in L^2$ and $g=\boldsymbol{C}_\omega f$, i.e.*

$$g(t)=\int\limits_{\mathbb{R}} C_\omega(t-\tau)f(\tau)d\tau. \tag{2.22}$$

Then $g\in L^2$, and the Fourier–Plancherel transforms $\hat{f}$, $\hat{g}$ of functions f and g are related by the equality

$$\hat{g}(\lambda)=\widehat{C_\omega}(\lambda)\cdot\hat{f}(\lambda), \quad \text{a.e. on } \mathbb{R}, \tag{2.23}$$

where $\widehat{C_\omega}(\lambda)$ is determined by the equality (2.14).

Proof. Lemma 2.4 is a direct consequence of Lemma 2.1. □

Lemma 2.5. *Let $f\in L^2$ and $g=\boldsymbol{S}_\omega f$, i.e.,*

$$g(t)=\text{p.v.}\int\limits_{\mathbb{R}} S_\omega(t-\tau)f(\tau)d\tau. \tag{2.24}$$

Then $g\in L^2$, and the Fourier–Plancherel transforms $\hat{f}$, $\hat{g}$ of functions f and g are related by the equality

$$\hat{g}(\lambda)=\widehat{S_\omega}(\lambda)\cdot\hat{f}(\lambda), \quad \text{a.e. on } \mathbb{R}, \tag{2.25}$$

where $\widehat{S_\omega}(\lambda)$ is determined by the equality (2.17).

Proof. Since $S_\omega \notin L^1$, Lemma 2.5 does not follow from Lemma 2.1 directly. Let

$$S_{\omega,\varepsilon}(t) = \begin{cases} S_\omega(t), & \text{if } t \in \mathbb{R} \setminus (-\varepsilon, \varepsilon), \\ 0 \quad , & \text{if } t \in (-\varepsilon, \varepsilon). \end{cases} \tag{2.26}$$

The function $S_{\omega,\varepsilon}$ belongs to L^1 for every $\varepsilon > 0$. Let

$$g_\varepsilon(t) = \int\limits_{\mathbb{R}} S_{\omega,\varepsilon}(t-\tau) f(\tau) d\tau. \tag{2.27}$$

Applying Lemma 2.1 to $k = S_{\omega,\varepsilon}$, we conclude that $g_\varepsilon \in L^2$ for every $\varepsilon > 0$ and that the Fourier–Plancherel transforms $\widehat{g_\varepsilon}$, $\widehat{f}$ of the functions g_ε, f are related by the equality

$$\widehat{g_\varepsilon}(\lambda) = \widehat{S_{\omega,\varepsilon}}(\lambda) \cdot \hat{f}(\lambda), \tag{2.28}$$

where $\widehat{S_{\omega,\varepsilon}}(\lambda)$ is defined by (2.15). According to Lemma 2.3,

$$\widehat{g_\varepsilon}(\lambda) = \widehat{S_\omega}(\lambda) \cdot \hat{f}(\lambda) - h_\varepsilon(\lambda), \tag{2.29}$$

where

$$h_\varepsilon(\lambda) = \varrho_\omega(\lambda, \varepsilon) \hat{f}(\lambda), \tag{2.30}$$

and the family $\{\varrho_\omega(\lambda, \varepsilon)\}_{0<\varepsilon<\infty}$ satisfies the conditions (2.19) and (2.20). From (2.19), (2.20), (2.30) and the Lebesgue Dominated Convergence Theorem, it follows that

$$\lim_{\varepsilon \to +0} \int\limits_{\mathbb{R}} |h_\varepsilon(\lambda)|^2 d\lambda = 0.$$

In other words,

$$\|\widehat{g_\varepsilon}(\lambda) - \hat{g}\|_{L^2} = 0, \tag{2.31}$$

where

$$\hat{g} \overset{\text{def}}{=} \widehat{S_\omega}(\lambda) \cdot \hat{f}(\lambda). \tag{2.32}$$

From (2.31) it follows that $\|g_\varepsilon - \check{g}\|_{L^2} \to 0$ as $\varepsilon \to +0$, i.e.,

$$\|S_{\omega,\varepsilon} f - \check{g}\|_{L^2} \to 0 \quad \text{as } \varepsilon \to +0, \tag{2.33}$$

where $\check{g} = \mathfrak{F}^{-1} \hat{g} \in L^2$. From the other side, $(S_{\omega,\varepsilon} f)(t) \to g(t)$ for a.e. $t \in \mathbb{R}$ by Lemma 1.4. Hence $g = \check{g}$, and $\hat{g} = \widehat{S_\omega} \hat{f}$. □

6. The equality

$$\left|\widehat{C_\omega}(\lambda)\right|^2 + \left|\widehat{S_\omega}(\lambda)\right|^2 = 1, \quad \forall\, \lambda \in \mathbb{R}, \tag{2.34}$$

plays a crucial role in this paper. This equation is a direct consequence of the explicit expressions (2.14) and (2.17) for $\widehat{C_\omega}$ and $\widehat{S_\omega}$ and the identity

$$(\cosh \zeta)^2 - (\sinh \zeta)^2 = 1, \quad \forall \zeta \in \mathbb{C}. \tag{2.35}$$

Lemma 2.6. *The operators $\boldsymbol{C}_\omega$ and $\boldsymbol{S}_\omega$ are contractive in the space $L^2(\mathbb{R})$. Moreover, the equality*

$$\|\boldsymbol{C}_\omega f\|^2_{L^2} + \|\boldsymbol{S}_\omega f\|^2_{L^2} = \|f\|^2_{L^2}, \quad \forall\, f \in L^2, \tag{2.36}$$

holds.

Proof. Let $g_c = \boldsymbol{C}_\omega f$, $g_s = \boldsymbol{S}_\omega f$ and let $\hat{f}$, $\widehat{g_c}$, $\widehat{g_s}$ be the Fourier–Plancherel transforms of the functions f, g_c, g_s. According to Lemmas 2.4 and 2.5, the equalities

$$\widehat{g_c}(\lambda) = \widehat{C_\omega}(\lambda)\hat{f}(\lambda), \quad \widehat{g_s}(\lambda) = \widehat{S_\omega}(\lambda)\hat{f}(\lambda), \quad \text{for a.e. } \lambda \in \mathbb{R}$$

hold. From (2.34) it follows that

$$|\widehat{g_c}(\lambda)|^2 + |\widehat{g_s}(\lambda)|^2 = |\hat{f}(\lambda)|^2, \quad \text{for a.e. } \lambda \in \mathbb{R}.$$

Integrating with respect to λ, we obtain the equality $\|\widehat{g_c}\|^2_{L^2} + \|\widehat{g_s}\|^2_{L^2} = \|\hat{f}\|^2_{L^2}$. In view of (2.6), the last equality is equivalent to the equality (2.36). □

3. The Akhiezer operators $\boldsymbol{\Phi}_\omega$ and $\boldsymbol{\Psi}_\omega$ in $L^2 \oplus L^2$

Definition 3.1. *The space $L^2 \oplus L^2$ is the set of all 2×1 columns $\boldsymbol{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$* such that $x_1(t) \in L^2$ and $x_2(t) \in L^2$. The set $L^2 \oplus L^2$ is equipped by the natural linear operations and by the inner product $\langle\,,\,\rangle_{L^2\oplus L^2}$. If $\boldsymbol{x'}(t) = \begin{bmatrix} x'_1(t) \\ x'_2(t) \end{bmatrix}$ and $\boldsymbol{x''}(t) = \begin{bmatrix} x''_1(t) \\ x''_2(t) \end{bmatrix}$ belong to $L^2 \oplus L^2$, then

$$\langle \boldsymbol{x'}, \boldsymbol{x''}\rangle_{L^2\oplus L^2} \stackrel{\text{def}}{=} \langle x'_1, x''_1\rangle_{L^2} + \langle x'_2, x''_2\rangle_{L^2}. \tag{3.1}$$

The inner product (3.1) generates the norm

$$\|\boldsymbol{x}\|_{L^2\oplus L^2} = \sqrt{\|x_1\|^2_{L^2} + \|x_2\|^2_{L^2}} \quad \text{for} \quad \boldsymbol{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \in L^2 \oplus L^2. \tag{3.2}$$

Since[2] $L^2 \subset L^1_\omega$, also $L^2 \oplus L^2 \subset L^1_\omega \dotplus L^1_\omega$. Thus if $\boldsymbol{x} \in L^2 \oplus L^2$, then the values $\boldsymbol{y}(t) = (\boldsymbol{\Phi}_\omega \boldsymbol{x})(t)$ and $\boldsymbol{z}(t) = (\boldsymbol{\Psi}_\omega \boldsymbol{x})(t)$ are defined by (1.16) for almost every $t \in \mathbb{R}$. Using Lemmas 2.4 and 2.5, we conclude from (1.16) that the operators $\boldsymbol{\Phi}_\omega$ and $\boldsymbol{\Psi}_\omega$ are bounded operators in the space $L^2 \oplus L^2$. In particular, the values $\boldsymbol{y}(t)$ and $\boldsymbol{z}(t)$ belong to $L^2 \oplus L^2$.

Theorem 3.2. *Each of the operators $\boldsymbol{\Phi}_\omega$ and $\boldsymbol{\Psi}_\omega$ is an isometric operator in the space $L^2 \oplus L^2$:*

$$\|\boldsymbol{\Phi}_\omega \boldsymbol{x}\|_{L^2\oplus L^2} = \|\boldsymbol{x}\|_{L^2\oplus L^2}, \quad \|\boldsymbol{\Psi}_\omega \boldsymbol{x}\|_{L^2\oplus L^2} = \|\boldsymbol{x}\|_{L^2\oplus L^2}, \quad \forall\, \boldsymbol{x} \in L^2 \oplus L^2. \tag{3.3}$$

[2] See (2.21).

Theorem 3.3. *The operators* $\mathbf{\Phi}_\omega$ *and* $\mathbf{\Psi}_\omega$ *are mutually inverse in the space* $L^2 \oplus L^2$*:*

$$\mathbf{\Psi}_\omega \mathbf{\Phi}_\omega \boldsymbol{x} = \boldsymbol{x}, \quad \forall\, \boldsymbol{x} \in L^2 \oplus L^2, \tag{3.4}$$

$$\mathbf{\Phi}_\omega \mathbf{\Psi}_\omega \boldsymbol{x} = \boldsymbol{x}, \quad \forall\, \boldsymbol{x} \in L^2 \oplus L^2. \tag{3.5}$$

Proofs of Theorem 3.2. Let us associate the 2×2 matrix functions $\widehat{\Phi_\omega}(\lambda)$ and $\widehat{\Psi_\omega}(\lambda)$ with the operators $\mathbf{\Phi}_\omega$ and $\mathbf{\Psi}_\omega$:

$$\widehat{\Phi_\omega}(\lambda) = \begin{bmatrix} \widehat{C_\omega}(\lambda) & \widehat{S_\omega}(\lambda) \\ \widehat{S_\omega}(\lambda) & \widehat{C_\omega}(\lambda) \end{bmatrix}, \quad \lambda \in \mathbb{R}, \tag{3.6a}$$

$$\widehat{\Psi_\omega}(\lambda) = \begin{bmatrix} \widehat{C_\omega}(\lambda) & -\widehat{S_\omega}(\lambda) \\ -\widehat{S_\omega}(\lambda) & \widehat{C_\omega}(\lambda) \end{bmatrix}, \quad \lambda \in \mathbb{R}, \tag{3.6b}$$

where $\widehat{C_\omega}(\lambda)$ and $\widehat{S_\omega}(\lambda)$ are the same that in (2.14) and (2.17). Let

$$\boldsymbol{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \in L^2 \oplus L^2, \quad \boldsymbol{y} = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \mathbf{\Phi}_\omega \boldsymbol{x},$$

and let $\widehat{\boldsymbol{x}} = \begin{bmatrix} \widehat{x_1} \\ \widehat{x_2} \end{bmatrix}$, $\widehat{\boldsymbol{y}} = \begin{bmatrix} \widehat{y_1} \\ \widehat{y_2} \end{bmatrix}$, where $\widehat{x_1}, \widehat{x_2}, \widehat{y_1}, \widehat{y_2}$ are the Fourier–Plancherel transforms of the functions x_1, x_2, y_1, y_2, respectively. According to the equality (1.16) and to Lemmas 2.4 and 2.5, the equality

$$\widehat{\boldsymbol{y}}(\lambda) = \widehat{\Phi_\omega}(\lambda)\widehat{\boldsymbol{x}}(\lambda) \tag{3.7}$$

holds for almost every $\lambda \in \mathbb{R}$.

From the equality (2.34) it follows that the matrix $\widehat{\Phi_\omega}(\lambda)$ is unitary for each $\lambda \in \mathbb{R}$:

$$\big(\widehat{\Phi_\omega}(\lambda)\big)^* \widehat{\Phi_\omega}(\lambda) = I, \quad \forall\, \lambda \in \mathbb{R}, \tag{3.8}$$

where I is 2×2 identity matrix. From (3.7) and (3.8) it follows that

$$\big(\widehat{\boldsymbol{y}}(\lambda)\big)^* \widehat{\boldsymbol{y}}(\lambda) = \big(\widehat{\boldsymbol{x}}(\lambda)\big)^* \widehat{\boldsymbol{x}}(\lambda), \quad \text{for a.e. } \lambda \in \mathbb{R},$$

i.e.,

$$|\widehat{y_1}(\lambda)|^2 + |\widehat{y_2}(\lambda)|^2 = |\widehat{x_1}(\lambda)|^2 + |\widehat{x_2}(\lambda)|^2, \quad \text{for a.e. } \lambda \in \mathbb{R}.$$

Integrating with respect to λ over $\mathbb{R}$ and using the Parseval identity (2.6), we conclude that

$$\|y_1\|^2_{L^2} + \|y_2\|^2_{L^2} = \|x_1\|^2_{L^2} + \|x_2\|^2_{L^2},$$

that is, $\|\mathbf{\Phi}_\omega \boldsymbol{x}\|_{L^2 \oplus L^2} = \|\boldsymbol{x}\|_{L^2 \oplus L^2}$. The equality $\|\mathbf{\Psi}_\omega \boldsymbol{x}\|_{L^2 \oplus L^2} = \|\boldsymbol{x}\|_{L^2 \oplus L^2}$ can be obtained analogously. □

Proof of Theorem 3.3. Let

$$\boldsymbol{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \in L^2 \oplus L^2, \quad \boldsymbol{y} = \begin{bmatrix} y_1 \\ y_2 \end{bmatrix} = \mathbf{\Phi}_\omega \boldsymbol{x}, \quad \boldsymbol{z} = \begin{bmatrix} z_1 \\ z_2 \end{bmatrix} = \mathbf{\Psi}_\omega \boldsymbol{y}.$$

Let $\widehat{\boldsymbol{x}} = \begin{bmatrix}\widehat{x_1}\\ \widehat{x_2}\end{bmatrix}$, $\widehat{\boldsymbol{y}} = \begin{bmatrix}\widehat{y_1}\\ \widehat{y_2}\end{bmatrix}$, $\widehat{\boldsymbol{z}} = \begin{bmatrix}\widehat{z_1}\\ \widehat{z_2}\end{bmatrix}$, where $\widehat{x_1}, \widehat{x_2}, \widehat{y_1}, \widehat{y_2}, \widehat{z_1}, \widehat{z_2}$ are the Fourier–Plancherel transforms of the functions $x_1, x_2, y_1, y_2, z_1, z_2$, respectively. We already proved the equality (3.7). In the same way the equality

$$\widehat{\boldsymbol{z}}(\lambda) = \widehat{\Psi_\omega}(\lambda)\widehat{\boldsymbol{y}}(\lambda), \quad \text{for a.e. } \lambda \in \mathbb{R}, \tag{3.9}$$

can be established. From (3.7) and (3.9) it follows that

$$\widehat{\boldsymbol{z}}(\lambda) = \widehat{\Psi_\omega}(\lambda)\widehat{\Phi_\omega}(\lambda)\widehat{\boldsymbol{x}}(\lambda), \quad \text{for a.e. } \lambda \in \mathbb{R}. \tag{3.10}$$

From the equality (2.34) it follows that the matrices $\Phi_\omega(\lambda)$ and $\Psi_\omega(\lambda)$ are mutually inverse:

$$\Phi_\omega(\lambda)\Psi_\omega(\lambda) = I, \quad \forall\, \lambda \in \mathbb{R}, \tag{3.11}$$

where I is 2×2 identity matrix. From (3.10) and (3.11) we conclude that

$$\widehat{\boldsymbol{z}}(\lambda) = \widehat{\boldsymbol{x}}(\lambda), \quad \text{for a.e. } \lambda \in \mathbb{R}.$$

Finally, $\boldsymbol{z} = \boldsymbol{x}$.

Equality (3.4) is proved. Equality (3.5) can be proved in the same way. □

4. The Hilbert transform

Definition 4.1. Let $u(\tau)$ be a complex-valued function which is defined for almost every $\tau \in \mathbb{R}$. We assume that the function u satisfies the condition

$$\int\limits_{\mathbb{R}} \frac{|u(\tau)|}{1+|\tau|} d\tau < \infty. \tag{4.1}$$

Then the integral

$$H_\varepsilon u(t) = \frac{1}{\pi} \int\limits_{\mathbb{R}\setminus(t-\varepsilon, t+\varepsilon)} \frac{u(\tau)}{t-\tau} d\tau \tag{4.2}$$

exists for every $t \in \mathbb{R}$ and $\varepsilon > 0$. For each $\varepsilon > 0$, the function $H_\varepsilon u(t)$ is a continuous function of t for $t \in \mathbb{R}$. The function $Hu(t)$ is defined for those $t \in \mathbb{R}$ for which the value $H_\varepsilon u(t)$ tends to a finite limit as $\varepsilon \to +0$:

$$Hu(t) \overset{\text{def}}{=} \lim_{\varepsilon \to +0} \frac{1}{\pi} \int\limits_{\mathbb{R}\setminus(t-\varepsilon, t+\varepsilon)} \frac{u(\tau)}{t-\tau} d\tau. \tag{4.3}$$

The function Hu is said to be the Hilbert transform of the function u.

Theorem 4.2 (A. I. Plessner). *Let $u(\tau)$ be a function which is defined for almost every $\tau \in \mathbb{R}$. If the function $u(\tau)$ satisfies the condition* (4.1)*, then its Hilbert transform $Hu(t)$ exists for almost every $t \in \mathbb{R}$.*

Proof. Proof of this Plessner's theorem can be found in [2, Theorem 100]. □

If u is a function from L^2, then u satisfies the condition (4.1). By Plessner's theorem, the Hilbert transform $v(t) = (Hu)(t)$ exists for almost every $t \in \mathbb{R}$.

Theorem 4.3 (E. C. Titchmarch). *Let u be a function from L^2. Then:*

1. *Its Hilbert transform $v = Hu$ also belongs to L^2, and the equality*
$$\|v\|_{L^2} = \|u\|_{L^2} \tag{4.4}$$
holds.
2. *The equality*
$$(Hv)(t) = -u(t) \tag{4.5}$$
holds for almost every $t \in \mathbb{R}$.

This theorem means that the Hilbert transform, considered as an operator in L^2, is an unitary operator which satisfies the equality
$$H^2 = -I, \tag{4.6}$$
where I is the identity operator in L^2.

Proof of Lemma 1.4. We use the decomposition (1.11) of the kernel $S(t-\tau)$ into the sum of the Hilbert kernel $\dfrac{1}{\pi(t-\tau)}$ and the "regular" kernel $r(t-\tau)$. Let $(a,b) \subset \mathbb{R}$ be an *arbitrary* finite interval of the real axis. We split the function $f(\tau)$ into the sum of two summands.
$$f(\tau) = g(\tau) + h(\tau), \tag{4.7}$$
where
$$g(\tau) = \begin{cases} f(\tau), & \text{if } \tau \in (a,b), \\ \ \ 0 \ \ , & \text{if } \tau \in \mathbb{R} \setminus (a,b). \end{cases} \tag{4.8}$$
So
$$h(\tau) = 0, \quad \text{if } \tau \in (a,b). \tag{4.9}$$
According to (1.11) and (4.7), the equality
$$\int\limits_{\mathbb{R}\setminus(t-\varepsilon,t+\varepsilon)} S_\omega(t-\tau)f(\tau)d\tau = I_{1,\varepsilon}(t) + I_{2,\varepsilon}(t) + I_{3,\varepsilon}(t) \tag{4.10}$$
holds, where
$$I_{1,\varepsilon}(t) = \int\limits_{\mathbb{R}\setminus(t-\varepsilon,t+\varepsilon)} \frac{1}{\pi(t-\tau)} g(\tau)d\tau, \tag{4.11}$$
$$I_{2,\varepsilon}(t) = \int\limits_{\mathbb{R}\setminus(t-\varepsilon,t+\varepsilon)} r(t-\tau)g(\tau)d\tau, \tag{4.12}$$
$$I_{3,\varepsilon}(t) = \int\limits_{\mathbb{R}\setminus(t-\varepsilon,t+\varepsilon)} S_\omega(t-\tau)h(\tau)d\tau. \tag{4.13}$$

Function g satisfies the condition (4.1). According Plessner's Theorem, $\lim\limits_{\varepsilon\to+0} I_{1,\varepsilon}(t)$ exists for almost every $t \in \mathbb{R}$. Since the function g is finitely supported and the kernel $r(t-\tau)$ is continuous, $\lim\limits_{\varepsilon\to+0} I_{2,\varepsilon}(t)$ exists for every $t \in \mathbb{R}$. Since the function $h(\tau)$ vanishes for $\tau \in (a,b)$ and $\int\limits_{\mathbb{R}} \frac{|h(\tau)|}{\cosh\omega\tau} d\tau < \infty$, $\lim\limits_{\varepsilon\to+0} I_{3,\varepsilon}(t)$ exists for every $t \in (a,b)$. In view of (4.10), the limit in (1.13) exists for almost every $t \in (a,b)$. Since (a,b) is an arbitrary finite interval, the limit in (1.13) exists for almost every $t \in \mathbb{R}$. □

5. The operators $\boldsymbol{C}_\omega$ and $\boldsymbol{S}_\omega$ in $\boldsymbol{L^2_\sigma}$

In this section we consider the operators $\boldsymbol{C}_\omega$ and $\boldsymbol{S}_\omega$ acting in spaces of functions growing slower than $e^{\omega|t|}$ as $t \to \pm\infty$.

Definition 5.1. For $\sigma \in \mathbb{R}$, the space L^2_σ is the space of all functions x which are measurable, defined almost everywhere with respect to the Lebesgue measure and satisfy the condition $\|x\|_{L^2_\sigma} < \infty$, where

$$\|x\|_{L^2_\sigma} = \Big\{ \int\limits_{\mathbb{R}} |x(\tau)|^2 e^{-2\sigma|\tau|} d\tau \Big\}^{1/2}. \tag{5.1}$$

The space L^2_σ is equipped by the standard linear operations and by the norm (5.1).

It is clear that the space L^2 which appeared in Sect. 2 is the space L^2_0, that is, L^2_σ with $\sigma = 0$.

In Sect. 1 we already have defined the functions $\boldsymbol{C}_\omega x$ and $\boldsymbol{S}_\omega x$ for x from the space L^1_ω. For $\sigma < \omega$, the space L^2_σ is contained in L^1_ω. If $x \in L^2_\sigma$, then

$$\int\limits_{\mathbb{R}} |x(t)| e^{-\omega|t|} dt \le \Big\{ \int\limits_{\mathbb{R}} |x(t)|^2 e^{-2\sigma|t|} dt \Big\}^{1/2} \Big\{ \int\limits_{\mathbb{R}} e^{-2(\omega-\sigma)|t|} dt \Big\}^{1/2} < \infty. \tag{5.2}$$

According to Lemmas 1.2 and 1.4, if $f \in L^1_\omega$, then the function $(\boldsymbol{C}_\omega f)(t)$ is defined for every $t \in \mathbb{R}$ and the function $(\boldsymbol{S}_\omega f)(t)$ is defined for almost every $t \in \mathbb{R}$.

In Sect. 2 we obtained that if $f \in L^2$, than $\boldsymbol{C}_\omega f \in L^2$ and $\boldsymbol{S}_\omega f \in L^2$. Moreover, we proved that the operators $\boldsymbol{C}_\omega$ and $\boldsymbol{S}_\omega$ are contractive in L^2; see Corollary 2.6. In this section we show that if $0 < \sigma < \omega$ and $f \in L^2_\sigma$, than $\boldsymbol{C}_\omega f \in L^2_\sigma$ and $\boldsymbol{S}_\omega f \in L^2_\sigma$. Moreover, we show that the operators $\boldsymbol{C}_\omega$ and $\boldsymbol{S}_\omega$ are bounded in the space L^2_σ.

Lemma 5.2. *Assume that* $0 \le \sigma < \omega$. *Let* $f \in L^2_\sigma$, *and* g *is related to* f *by means of the formula* (2.22), *i.e.,* $g = \boldsymbol{C}_\omega f$. *Then* $g \in L^2_\sigma$, *and*

$$\|g\|_{L^2_\sigma} \le \frac{M_c}{1-\sigma/\omega} \, \|f\|_{L^2_\sigma}, \tag{5.3}$$

where $M_c < \infty$ *is a value which does not depend on* ω *and* σ.

Proof. Let

$$u(\tau) = f(\tau)e^{-\sigma|\tau|}, \quad v(t) = g(t)e^{-\sigma|t|}. \tag{5.4}$$

Since $f \in L^2_\sigma$, $u \in L^2$. Equality (2.22) can be rewritten as

$$v(t) = \int\limits_{\mathbb{R}} e^{-\sigma|t|+\sigma|\tau|} C_\omega(t-\tau)u(\tau)d\tau. \tag{5.5}$$

Let us estimate the kernel

$$K_c(t,\tau) = e^{-\sigma|t|+\sigma|\tau|}\, C_\omega(t-\tau). \tag{5.6}$$

For $\sigma \geq 0$ the inequality

$$\big| -\sigma|t| + \sigma|\tau|\big| \leq \sigma|t-\tau|, \quad \forall\, t \in \mathbb{R},\, \tau \in \mathbb{R}, \tag{5.7}$$

holds. Hence

$$e^{-\sigma|t|+\sigma|\tau|} \leq e^{\sigma|t-\tau|}, \quad \forall\, t \in \mathbb{R},\, \tau \in \mathbb{R}. \tag{5.8}$$

From this inequality and from the expression (1.4) for C_ω we conclude that

$$|K_c(t,\tau) \leq k^c_{\sigma,\omega}(t-\tau), \quad \forall\, t \in \mathbb{R},\, \tau \in \mathbb{R}, \tag{5.9}$$

where

$$k^c_{\sigma,\omega}(\xi) = \frac{\omega}{\pi}\frac{e^{\sigma|\xi|}}{\cosh \omega\xi}, \quad \xi \in \mathbb{R}. \tag{5.10}$$

For $0 \leq \sigma < \omega$, the function $k^c_{\sigma,\omega}$ belongs to L^1 and

$$\|k^c_{\sigma,\omega}\|_{L_1} < \frac{4}{\pi}\int\limits_0^\infty \frac{\cosh a\xi}{\cosh \xi} d\xi\,, \tag{5.11}$$

where

$$a = \frac{\sigma}{\omega}\cdot \tag{5.12}$$

The integral in (5.11) can be calculated explicitly:

$$\int\limits_0^\infty \frac{\cosh a\xi}{\cosh \xi} d\xi = \frac{\pi}{2\cos\frac{\pi}{2}a}\cdot \tag{5.13}$$

Thus

$$\|k^c_{\sigma,\omega}\|_{L_1} < \frac{2}{\sin\frac{\pi}{2}(1-a)}\cdot \tag{5.14}$$

Since $\sin\frac{\pi}{2}\eta \geq \eta$ for $0 \leq \eta \leq 1$, inequality (5.14) implies the inequality

$$\|k^c_{\sigma,\omega}\|_{L^1} < \frac{2}{1-\sigma/\omega}. \tag{5.15}$$

From (5.5) and (5.9) we obtain the inequality $|v(t)| \leq w(t)$, $\forall\, t \in \mathbb{R}$, and

$$\|v\|_{L^2} \leq \|w\|_{L^2}, \tag{5.16}$$

where

$$w(t) = \int\limits_{\mathbb{R}} k^c_{\sigma,\omega}(t-\tau)|u(\tau)|d\tau. \tag{5.17}$$

According to Lemma 2.1, $w \in L^2$, and the inequality

$$\|w\|_{L^2} \leq \|k^c_{\sigma,\omega}\|_{L^1} \cdot \|u\|_{L^2} \tag{5.18}$$

holds. The inequality

$$\|v\|_{L^2} \leq \frac{2}{1-\sigma/\omega}\,\|u\|_{L_2}$$

is a consequence of the equalities (5.16), (5.18), and (5.15). According to (5.4), $\|u\|_{L^2} = \|f\|_{L^2_\sigma}$, $\|v\|_{L^2} = \|g\|_{L^2_\sigma}$. So the inequality (5.3) holds with $M_c = 2$. $\square$

Lemma 5.3. *Assume that* $0 \leq \sigma < \omega$. *Let* $f \in L^2_\sigma$, *and* g *is related to* f *by means of the formula* (2.24), *i.e.,* $g = \boldsymbol{S}_\omega f$. *Then* $g \in L^2_\sigma$, *and*

$$\|g\|_{L^2_\sigma} \leq \frac{M_s}{(1-\sigma/\omega)^2}\,\|f\|_{L^2_\sigma}, \tag{5.19}$$

where $M_s < \infty$ *is a value which does not depend on* ω *and* σ.

Proof. Let $u(\tau)$, $v(t)$ be defined according to (5.4). Since $f \in L^2_\sigma$, $u \in L^2$. The equality (2.24) can be rewritten as

$$v(t) = \text{p.v.} \int\limits_{\mathbb{R}} e^{-\sigma|t|+\sigma|\tau|} S_\omega(t-\tau)u(\tau)d\tau. \tag{5.20}$$

We present $v(t)$ as

$$v(t) = v_1(t) + v_2(t), \tag{5.21}$$

where

$$v_1(t) = \text{p.v.} \int\limits_{\mathbb{R}} S_\omega(t-\tau)u(\tau)d\tau, \tag{5.22}$$

$$v_2(t) = \int\limits_{\mathbb{R}} (e^{-\sigma|t|+\sigma|\tau|} - 1) S_\omega(t-\tau)u(\tau)d\tau, \tag{5.23}$$

Let us estimate the kernel

$$K_s(t,\tau) = (e^{-\sigma|t|+\sigma|\tau|} - 1)S_\omega(t-\tau). \tag{5.24}$$

From the inequalities $|e^\xi - 1| \leq |\xi| e^{|\xi|}$, from (5.7) and from the expression (1.4) for S_ω we conclude that

$$|K_s(t,\tau)| \leq k^s_{\sigma,\omega} s(t-\tau), \tag{5.25}$$

where

$$k^s_{\sigma,\omega}(\xi) = \frac{\omega}{\pi} \cdot \frac{\sigma|\xi|\, e^{\sigma|\xi|}}{\sinh \omega|\xi|}. \tag{5.26}$$

The function $k^s_{\sigma,\omega}$ belongs to L^1, and

$$\|k^s_{\sigma,\omega}\|_{L_1} < \frac{4a}{\pi} \int\limits_0^\infty \frac{\xi\, \cosh a\xi}{\sinh \xi}, \tag{5.27}$$

where a is the same that in (5.12). The integral in (5.27) can be calculated explicitly:

$$\int_0^\infty \frac{\xi \cosh a\xi}{\sinh \xi} d\xi = \frac{\pi^2}{4\sin^2 \frac{\pi}{2}(1-a)}. \tag{5.28}$$

Thus the inequality

$$\|k^s_{\sigma,\omega}\|_{L^1} < \frac{\pi}{(1-\sigma/\omega)^2} \tag{5.29}$$

holds. From (5.23), (5.24), and (5.25) it follows that

$$\|v_2\|_{L^2} \leq \|w\|_{L^2}, \tag{5.30}$$

where

$$w(t) = \int_{\mathbb{R}} k^s_{\sigma,\omega}(t-\tau)|u(\tau)|d\tau. \tag{5.31}$$

According to Lemma 2.1, $w \in L^2$, and the inequality

$$\|w\|_{L^2} \leq \|k^s_{\sigma,\omega}\|_{L^1} \cdot \|u\|_{L^2} \tag{5.32}$$

holds. From (5.29), (5.32), and (5.30) we conclude that

$$\|v_2\|_{L^2} \leq \frac{\pi}{(1-\sigma/\omega)^2}\|u\|_{L^2}. \tag{5.33}$$

According to Lemma 2.6, the inequality

$$\|v_1\|_{L^2} \leq \|u\|_{L^2} \tag{5.34}$$

holds. From (5.21), (5.34), and (5.33) we derive the inequality

$$\|v\|_{L^2} \leq \frac{M_s}{(1-\sigma/\omega)^2}\|u\|_{L^2} \tag{5.35}$$

with $M_s = \pi + 1$. □

6. The Akhiezer operators Φ_ω and Ψ_ω in $L^2_\sigma \oplus L^2_\sigma$

Definition 6.1. *The space* $L^2_\sigma \oplus L^2_\sigma$ is the set of all 2×1 columns $\boldsymbol{x} = \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$ such that $x_1(t) \in L^2_\sigma$ and $x_2(t) \in L^2_\sigma$, where L^2_σ was defined in Definition 5.1. The set $L^2_\sigma \oplus L^2_\sigma$ is equipped by the natural linear operations and by the norm

$$\|\boldsymbol{x}\|_{L^2_\sigma \oplus L^2_\sigma} = \sqrt{\|x_1\|^2_{L^2_\sigma} + \|x_2\|^2_{L^2_\sigma}}. \tag{6.1}$$

Since[3] $L^2_\sigma \subset L^1_\omega$, also $L^2_\sigma \oplus L^2_\sigma \subset L^1_\omega \dotplus L^1_\omega$. Thus if $\boldsymbol{x} \in L^2_\sigma \oplus L^2_\sigma$, then the values $\boldsymbol{y}(t) = (\boldsymbol{\Phi}_\omega \boldsymbol{x})(t)$ and $\boldsymbol{z}(t) = (\boldsymbol{\Psi}_\omega \boldsymbol{x})(t)$ are defined by (1.16) for almost every $t \in \mathbb{R}$. From Lemmas 5.2 and 5.3 we derive

[3] See (5.2).

Lemma 6.2. *We assume that* $0 \le \sigma < \omega$. *Let* $\boldsymbol{x} \in L^2_\sigma \oplus L^2_\sigma$ *and let* $\boldsymbol{y} = \boldsymbol{\Phi}_\omega \boldsymbol{x}$, $\boldsymbol{z} = \boldsymbol{\Psi}_\omega \boldsymbol{x}$ *be defined by* (1.16). *Then* $\boldsymbol{y} \in L^2_\sigma \oplus L^2_\sigma$, $\boldsymbol{z} \in L^2_\sigma \oplus L^2_\sigma$, *and the estimates hold*

$$\|\boldsymbol{\Phi}_\omega \boldsymbol{x}\|_{L^2_\sigma \oplus L^2_\sigma} \le \tfrac{M}{1-\sigma/\omega} \|\boldsymbol{x}\|_{L^2_\sigma \oplus L^2_\sigma}, \tag{6.2}$$

$$\|\boldsymbol{\Psi}_\omega \boldsymbol{x}\|_{L^2_\sigma \oplus L^2_\sigma} \le \tfrac{M}{1-\sigma/\omega} \|\boldsymbol{x}\|_{L^2_\sigma \oplus L^2_\sigma}, \tag{6.3}$$

where $M < \infty$ *is a value which does not depend on* σ, ω, $\boldsymbol{x}$.

The following theorem is the main result of this paper.

Theorem 6.3. *We assume that* $0 \le \sigma < \omega$. *Then for every* $\boldsymbol{x} \in L^2_\sigma \oplus L^2_\sigma$ *the equalities*

$$\boldsymbol{\Psi}_\omega \boldsymbol{\Phi}_\omega \boldsymbol{x} = \boldsymbol{x}, \quad \boldsymbol{\Phi}_\omega \boldsymbol{\Psi}_\omega \boldsymbol{x} = \boldsymbol{x} \tag{6.4}$$

hold.

Proof. From Lemma 6.2 it follows that operators $\boldsymbol{\Psi}_\omega \boldsymbol{\Phi}_\omega$ and $\boldsymbol{\Phi}_\omega \boldsymbol{\Psi}_\omega$ are bounded linear operators in the space $L^2_\sigma \oplus L^2_\sigma$. The set $L^2 \oplus L^2$ is a dense subset of the space $L^2_\sigma \oplus L^2_\sigma$. By Theorem 3.3, equalities (6.4) hold for every $\boldsymbol{x} \in L^2 \oplus L^2$. By continuity, equalities (6.4) can be extended from $L^2 \oplus L^2$ to $L^2_\sigma \oplus L^2_\sigma$. □

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On Gaussian random matrices coupled to the discrete Laplacian

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Abstract. We study operators obtained by coupling an $n \times n$ random matrix from one of the Gaussian ensembles to the discrete Laplacian. We find the joint distribution of the eigenvalues and resonances of such operators. This is one of the possible mathematical models for quantum scattering in a complex physical system with one semi-infinite lead attached.

1. Introduction

Given a random Hermitian $n \times n$ matrix $\mathcal{H}$ from one of the classical Gaussian ensembles, we consider the operator on $\ell^2(\mathbb{Z}_+)$ obtained from $\mathcal{H}$ by coupling it to the discrete Laplacian as follows:

$$\widetilde{\mathcal{H}} = \left(\begin{array}{c|ccc} \gamma\mathcal{H} & & & \\ & \kappa & & \\ \hline \kappa & 0 & 1 & \\ & 1 & 0 & \ddots \\ & & \ddots & \ddots \end{array}\right). \tag{1.1}$$

Here γ is any deterministic constant, and κ is either a random variable (independent of $\mathcal{H}$) with a given distribution or deterministic $\kappa = 1$.

Such an operator is natural from the point of view of physics: the random matrix part corresponds to a complex physical system of particles whose interactions are unknown, and the discrete Laplacian part corresponds to a lead attached via some coupling of strength κ.

We are interested in the spectral properties of the operator $\widetilde{\mathcal{H}}$, namely in the locations of its eigenvalues and resonances (see Sect. 2.1 below). In Theorem 3.1, which is our main result, we compute the joint distribution of eigenvalues and

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resonances of $\widetilde{\mathcal{H}}$ for the case of random κ. See remarks after the theorem for the case of deterministic $\kappa = 1$.

The proof involves two main steps: first, we apply the Dumitriu–Edelman [4, 24] tridiagonalization procedure to reduce $\widetilde{\mathcal{H}}$ to a Jacobi operator on $\ell^2(\mathbb{Z}_+)$; second, we employ the (suitably modified) Geronimo–Case equations [9] (see also Damanik–Simon [3, Appendix A]) to access the Jost function whose zeros determine the locations of eigenvalues and resonances.

Aside from the physical importance, interest to the resonances comes from the fact that the locations of eigenvalues and resonances allow to fully recover the spectral measure of our operator $\widetilde{\mathcal{H}}$. For the background on spectral theory of Jacobi operators we refer the reader to the monographs of Simon [22] and Teschl [23]. The resonance problem for Jacobi operators was the topic of [2, 3, 8, 9, 10, 11, 12, 16, 17, 19, 20], among many others. A closely related scattering theory for Jacobi operators is discussed in [23].

An operator-based approach to the asymptotics of the Dumitriu–Edelman Jacobi matrices was studied by Ramírez–Rider–Virág [21] and Valkó–Virág [25], see also subsequent papers by the same authors. There is also a vast literature on the Jacobi (or discrete Schrödinger) operators with random coefficients, in particular in connection to the Anderson model, which we will not attempt to review here.

Random matrix approach to open quantum systems has two other alternatives to $\widetilde{\mathcal{H}}$: through non-Hermitian perturbations of Hermitian random matrices and through non-unitary perturbations of unitary random matrices – see [5, 6, 7, 13] and references therein. Theory of orthogonal polynomials is applicable in both of these scenarios as well; see [14, 18].

The organization of the paper is as follows. In Sects. 2.1–2.3 we provide the background from the theory of Jacobi operators, including properties of resonances, the Jost function (perturbation determinant), and the Geronimo–Case equations. In Sect. 3 we state our main result and provide the proof.

2. Jacobi operators

2.1. Finite range operators and perturbation determinants

By a Jacobi operator we call a tridiagonal operator acting on $\ell^2(\mathbb{Z}_+)$ of the form

$$\mathcal{J}(\mathbf{a},\mathbf{b}) = \begin{pmatrix} b_1 & a_1 & 0 & \\ a_1 & b_2 & a_2 & \ddots \\ 0 & a_2 & b_3 & \ddots \\ & \ddots & \ddots & \ddots \end{pmatrix}, \tag{2.1}$$

where $\mathbf{a} = \{a_j\}_{j=1}^{\infty}$, $\mathbf{b} = \{b_j\}_{j=1}^{\infty}$ have $a_j > 0$ and $b_j \in \mathbb{R}$.

The case $\mathbf{a} = \{1\}_{j=1}^{\infty}$, $\mathbf{b} = \{0\}_{j=1}^{\infty}$ corresponds to $\mathcal{J}_0$, the discrete Laplacian on $\mathbb{Z}_+$, and will be referred to as the free Jacobi operator.

For $s \geq 0$, we denote by $\mathcal{T}^{[2s]}$ the set of all Jacobi operators that have $a_j = 1$, $b_j = 0$ for $j > s$ and $a_s \neq 1$. We denote by $\mathcal{T}^{[2s+1]}$ the set of all Jacobi operators that have $a_j = 1$, $b_j = 0$ for $j > s+1$, and $a_s = 1$, but $b_s \neq 0$. We denote $\mathcal{T}^{[k\geq 0]}$ to be the set of all Jacobi operators that are finite rank perturbations of the free one. It is the disjoint union of all $\mathcal{T}^{[k]}$, $k \geq 0$.

The spectral measure μ (with respect to the vector $\mathbf{e}_1 = (1,0,0,\dots)^T$) of an operator $\mathcal{J}$ (with bounded sequences $\mathbf{a}$ and $\mathbf{b}$) is defined to be the unique probability measure on $\mathbb{R}$ satisfying

$$\langle \mathbf{e}_1, \mathcal{J}^k \mathbf{e}_1 \rangle = \int_{\mathbb{R}} x^k \, d\mu(x), \qquad \text{for all } k \in \mathbb{Z}_+$$

(here $\langle \cdot, \cdot \rangle$ denotes the standard inner product in $\ell^2(\mathbb{Z}_+)$). If $\mathcal{J} \in \mathcal{T}^{[k\geq 0]}$ then its spectral measure is of the form (see [8, 3, 17])

$$d\mu(x) = \frac{\sqrt{4-x^2}}{a(x)} 1_{[-2,2]}(x)\, dx + d\mu_{p.p.} \tag{2.2}$$

where $a(x)$ is a polynomial and $\mu_{p.p.}$ contains finitely many pure points in $\mathbb{R}\setminus[-2,2]$ whose locations form a subset of the set of zeros of $a(x)$.

The m-function of $\mathcal{J}$,

$$m(z) = \int_{\mathbb{R}} \frac{d\mu(x)}{x-z},$$

is meromorphic in $\mathbb{C} \setminus [-2,2]$ with poles at the pure points of μ (eigenvalues of $\mathcal{J}$). By (2.2), m has a meromorphic continuation through $[-2,2]$ to a second copy of $\mathbb{C} \setminus [-2,2]$. Poles of m on this second sheet are typically referred to as the resonances of $\mathcal{J}$.

Let $\mathbb{D} = \{z : |z| < 1\}$. For $z \in \mathbb{C} \setminus \overline{\mathbb{D}}$, we define

$$M^*(z) = -m(z + z^{-1}).$$

From the arguments in the previous paragraph, M^* can be meromorphically continued from $\mathbb{C} \setminus \overline{\mathbb{D}}$ to $\mathbb{C}$. If $\mathcal{J} \in \mathcal{T}^{[k]}$ then M^* has precisely k poles in $\mathbb{C} \setminus \{0\}$ counted with multiplicity. Note that our $M^*(z)$ function is $M(1/z)$ in the notation of [3, 22].

For $\mathcal{J} \in \mathcal{T}^{[k]}$ let us define the perturbation determinant

$$L(z) = \det \left[(\mathcal{J} - z - z^{-1}))(\mathcal{J}_0 - z - z^{-1}))^{-1} \right], \qquad z \in \mathbb{D}.$$

(up to a normalization constant, $L(z)$ is equal to the Jost function of $\mathcal{J}$) Then $L(z)$ is a polynomial of degree k with $L(0) = 1$ (see, e.g., [15, Sect. 2] and [3, Appendix A]). It will be convenient to work with the following polynomial instead:

$$L^*(z) = z^k L(1/z).$$

Then for $\mathcal{J} \in \mathcal{T}^{[k]}$, $L^*(z)$ is a *monic* polynomial of degree k. It has zeros at the poles of M^* in $\mathbb{C} \setminus \{0\}$ counted with multiplicity.

Zeros z_j of L^* in $\mathbb{C}\setminus\overline{\mathbb{D}}$ are in one-to-one correspondence with the eigenvalues $z_j + z_j^{-1}$ of $\mathcal{J}$, and zeros z_j of L^* in $\overline{\mathbb{D}}\setminus\{0\}$ are in one-to-one correspondence with the resonances $z_j+z_j^{-1}$ of $\mathcal{J}$ (counted with multiplicity). In order to simplify presentation, we will therefore refer to zeros of L^* themselves as the eigenvalues, resp. resonances, of $\mathcal{J}$, with the post-application of the Joukowsky map $z\mapsto z+z^{-1}$ being implicitly understood.

2.2. Geronimo–Case equations

Let $\mathcal{J}\in\mathcal{T}^{[k]}$, μ be its spectral measure, and $P_n(z)$ $(n\geq 0)$ be the degree n monic orthogonal polynomial associated with μ. It is the characteristic polynomial of the top-left $n\times n$ corner of $\mathcal{J}$. For each $j\geq 0$ we define

$$K_{2j}(z) = K_{2j+1}(z) = z^j P_j(z+z^{-1}). \tag{2.3}$$

Note that $K_{2j}=K_{2j+1}$ is a monic polynomial of degree $2j$.

For each $0\leq j\leq k$, let $\hat{\mathcal{J}}_j$ be the unique Jacobi operator that maximizes the number of zero entries in $\mathcal{J}-\hat{\mathcal{J}}_j$ under the restriction that $\hat{\mathcal{J}}_j\in\mathcal{T}^{[j]}$. In particular, $\hat{\mathcal{J}}_0$ is the free Jacobi operator, and $\hat{\mathcal{J}}_k=\mathcal{J}$. Let $L_j^*(z)$ be the polynomial $L^*(z)$ (see the previous subsection) for the Jacobi operator $\hat{\mathcal{J}}_j$:

$$L_j^*(z) := L^*(z;\hat{\mathcal{J}}_j).$$

Recall that each L_j^* is monic and of degree j.

Then the system of polynomials $\{K_j, L_j^*\}$ satisfies the recurrence relation below, which we call the Geronimo–Case equations. They have been modified compared with [9, 3]: e.g., in the notation of [3], their $C_n(z)$ and $G_n(z)$ are ours $K_{2n}(z)$ and $z^{2n}L_{2n}^*(1/z)$, respectively. Taking this change into account, the Geronimo–Case equations [3, (A.19)] take the form

$$\begin{pmatrix} L_{2k+2}^*(z) \\ K_{2k+2}(z) \end{pmatrix} = \begin{pmatrix} z & -(a_{k+1}^2-1) \\ z & 1 \end{pmatrix} \begin{pmatrix} L_{2k+1}^*(z) \\ K_{2k+1}(z) \end{pmatrix} \tag{2.4}$$

and

$$\begin{pmatrix} L_{2k+1}^*(z) \\ K_{2k+1}(z) \end{pmatrix} = \begin{pmatrix} z & -b_{k+1} \\ 0 & 1 \end{pmatrix} \begin{pmatrix} L_{2k}^*(z) \\ K_{2k}(z) \end{pmatrix} \tag{2.5}$$

with the initial conditions $L_0^*(z)=K_0(z)=1$.

In the next lemma we collect some of the properties of polynomials L_j^*, K_j that we will need in Sect. 3 below.

Lemma 2.1. *For a given m, let*

$$L_m^*(z) = z^m + u_{m-1}z^{m-1} + u_{m-2}z^{m-2} + \cdots + u_1 z + u_0 = \prod_{j=1}^m (z-z_j).$$

Then

(i)

$$(-1)^m \prod_{j=1}^m z_j = u_0 = \begin{cases} 1-a_{m/2}^2 & \textit{if } m \bmod 2 = 0, \\ -b_{(m+1)/2} & \textit{if } m \bmod 2 = 1. \end{cases}$$

(ii)

$$-\sum_{j=1}^{m} z_j = -\sum_{j=1}^{\left\lfloor \frac{m+1}{2} \right\rfloor} b_j = u_{m-1}.$$

(iii)

$$\sum_{\substack{j,k=1\\ j<k}}^{m} z_j z_k = \sum_{\substack{j,k=1\\ j<k}}^{\left\lfloor \frac{m+1}{2} \right\rfloor} b_j b_k - \sum_{j=1}^{\left\lfloor \frac{m}{2} \right\rfloor} \left(a_j^2 - 1\right) = u_{m-2}.$$

(iv)

$$\sum_{j=1}^{m} z_j^2 = \sum_{j=1}^{\left\lfloor \frac{m+1}{2} \right\rfloor} b_j^2 + 2\sum_{j=1}^{\left\lfloor \frac{m}{2} \right\rfloor} \left(a_j^2 - 1\right) = u_{m-1}^2 - 2u_{m-2}.$$

(v)

$$\prod_{\substack{j,k=1\\ j<k}}^{m} (1 - z_j \bar{z}_k) \prod_{j=1}^{m} \frac{1}{1 - z_j^2} = \prod_{j=1}^{\left\lfloor \frac{m}{2} \right\rfloor} a_j^{4j}. \tag{2.6}$$

Proof. (i) Note that $K_j(0) = 1$, so this part follows immediately from (2.4) and (2.5) by plugging in $z = 0$.

(ii) Since K_{2k+1} is of degree $2k$, (2.4) shows that z^{2k+1}-coefficient of L_{2k+2}^* is equal to the z^{2k}-coefficient of L_{2k+1}^*. Equation (2.5) shows that z^{2k}-coefficient of L_{2k+1}^* is equal to the z^{2k-1}-coefficient of L_{2k}^* minus b_{k+1}. An induction on m then completes the proof.

Claim (iii) can be shown in the exact same way by considering the terms one degree lower.

Claim (iv) is immediate from (ii) and (iii) and $\sum z_j^2 = (\sum z_j)^2 - 2\sum_{j<k} z_j z_k$.

(v) For a polynomial p with real coefficients of degree j we define the operation $p^*(z) := z^j p(1/z)$. Then $(p^*)^* = p$, so we define $L_j(z) = (L_j^*)^*$. Using $K_j^* = K_j$ and the recurrences (2.4) and (2.5), we deduce

$$K_{2k}(z) = K_{2k+1}(z) = \frac{L_{2k}(z) - z^2 L_{2k}^*(z)}{1 - z^2} \tag{2.7}$$

and

$$K_{2k}(z) = K_{2k+1}(z) = \frac{L_{2k+1}(z) - z L_{2k+1}^*(z)}{1 - z^2}. \tag{2.8}$$

Let $\{z_j^{(k)}\}$ be the zeros of L_k^* and let $\{\lambda_j^{(k)}\}$ be the zeros of K_k. Denote the left-hand side of (2.6) by R_m. Then for $m = 2k$ even, we get

$$R_{2k} = \prod_{j=1}^{2k} \frac{L_{2k}\left(z_j^{(2k)}\right)}{1 - \left(z_j^{(2k)}\right)^2} = \prod_{j=1}^{2k} K_{2k}\left(z_j^{(2k)}\right)$$

by (2.7). This can be further rewritten as

$$R_{2k} = \prod_{j,s=1}^{2k} \big(z_j^{(2k)} - \lambda_s^{(2k)}\big) = \prod_{j=1}^{2k} L_{2k}^*\big(\lambda_j^{(2k)}\big) = \prod_{j=1}^{2k} \frac{1}{\lambda_j^{(2k)}} L_{2k+1}^*\big(\lambda_j^{(2k)}\big),$$

where we used (2.5). Note that $\prod_j^{(2k)} \lambda_j^{(2k)}$ is equal to the last coefficient of K_{2j} which is 1. So we get

$$R_{2k} = \prod_{j=1}^{2k} L_{2k+1}^*\big(\lambda_j^{(2k)}\big) = \prod_{j=1}^{2k+1} K_{2k}\big(z_j^{(2k+1)}\big) = \prod_{j=1}^{2k+1} \frac{L_{2k+1}\big(z_j^{(2k+1)}\big)}{1-\big(z_j^{(2k+1)}\big)^2} = R_{2k+1},$$

where we used (2.8).

For $m = 2k+1$, following analogous steps, we get:

$$\begin{aligned}
R_{2k+1} &= \prod_{j=1}^{2k+1} \frac{L_{2k+1}\big(z_j^{(2k+1)}\big)}{1-\big(z_j^{(2k+1)}\big)^2} = \prod_{j=1}^{2k+1} K_{2k+1}\big(z_j^{(2k+1)}\big) \\
&= \prod_{j=1}^{2k+1} \prod_{s=1}^{2k} \big(z_j^{(2k+1)} - \lambda_s^{(2k+1)}\big) = \prod_{j=1}^{2k} L_{2k+1}^*\big(\lambda_j^{(2k+1)}\big) \\
&= \prod_{j=1}^{2k} \frac{1}{\lambda_j^{(2k+1)}} L_{2k+2}^*\big(\lambda_j^{(2k+1)}\big) = \prod_{j=1}^{2k+2} K_{2k+1}\big(z_j^{(2k+2)}\big) \\
&= \prod_{j=1}^{2k+2} \frac{1}{a_{k+1}^2} K_{2k+2}\big(z_j^{(2k+2)}\big) = \frac{1}{a_{k+1}^{4(k+1)}} \prod_{j=1}^{2k+2} \frac{L_{2k+2}\big(z_j^{(2k+2)}\big)}{1-\big(z_j^{(2k+2)}\big)^2} \\
&= \frac{1}{a_{k+1}^{4(k+1)}} R_{2k+2},
\end{aligned}$$

where in the second to last line we used $a_{k+1}^2 K_{2k+1} = K_{2k+2} - L_{2k+2}^*$ which is a consequence of (2.4). Combining our recurrences for R_j's, we obtain (2.6). □

2.3. Locations of resonances and eigenvalues

It was shown in [3] that the set of resonances and eigenvalues of $\mathcal{J} \in \mathcal{T}^{[k\geq 0]}$ uniquely determines $\mathcal{J}$. In fact (see [17, Theorem 5.1]), the following sets $S(k)$ classify all possible configurations of resonances and eigenvalues of $\mathcal{J} \in \mathcal{T}^{[k]}$, $k \geq 0$.

Definition 2.2. *Denote by $S(k)$ the set of all possible $\{z_j\}_{j=1}^k$ in $(\mathbb{C}\setminus\{0\})^k$ that satisfy the following conditions:*

(i) *z_j's are real or come in complex-conjugate pairs, counted with multiplicity.*
(ii) *z_j's that lie in $\mathbb{C}\setminus\mathbb{D}$ are real and of multiplicity 1.*
(iii) *Let $1 < x_1 < x_2 < \cdots$ be the positive z_j's on $\mathbb{C}\setminus\overline{\mathbb{D}}$. Then*
  (a) *There is an even number of z_j's (counted with multiplicity) on $(x_1^{-1}, 1]$;*
  (b) *There is an odd number of z_j's (counted with multiplicity) on (x_{m+1}^{-1}, x_m^{-1}) $(m \geq 1)$;*

(c) *None of z_j's is equal to x_m^{-1} $(m \geq 1)$;*

(iv) *Let $\cdots < y_2 < y_1 < -1$ be the negative z_j's on $\mathbb{C} \setminus \overline{\mathbb{D}}$. Then*

(a) *There is an even number of z_j's (counted with multiplicity) on $[-1, y_1^{-1})$;*

(b) *There is an odd number of z_j's (counted with multiplicity) on (y_m^{-1}, y_{m+1}^{-1}) $(m \geq 1)$;*

(c) *None of z_j's is equal to y_m^{-1} $(m \geq 1)$.*

3. Random matrices coupled to the Laplacian

Let $N(0,1)$ be the real normal random variable with mean 0 and variance 1. Let Y be an $n \times n$ matrix with independent identically distributed real entries chosen from $N(0,1)$. Then we say that the random matrix $X = \frac{1}{2}(Y + Y^*)\frac{\sqrt{2}}{\sqrt{\beta n}}$ (where $\beta = 1$) belongs to the *Gaussian orthogonal ensemble.*

Similarly, let Y be an $n \times n$ matrix with independent identically distributed complex entries chosen from $N(0,1) + N(0,1)\mathrm{i}$. Then we say that the random matrix $X = \frac{1}{2}(Y + Y^*)\frac{\sqrt{2}}{\sqrt{\beta n}}$ (where $\beta = 2$) belongs to the *Gaussian unitary ensemble.*

Finally, let Y be an $n \times n$ matrix with independent identically distributed quternionic entries chosen from $N(0,1) + N(0,1)\mathrm{i} + N(0,1)\mathrm{j} + N(0,1)\mathrm{k}$. Then we say that the random matrix $X = \frac{1}{2}(Y + Y^R)\frac{\sqrt{2}}{\sqrt{\beta n}}$ (where $\beta = 4$) belongs to the *Gaussian symplectic ensemble.*

We denote these ensembles by GOE_n, GUE_n, GSE_n, respectively.

Note that we chose the extra scaling factor $\frac{\sqrt{2}}{\sqrt{\beta n}}$. This is chosen so that the empirical density of states of each of these ensembles converges to semicircle distribution $\frac{1}{2\pi}\sqrt{4 - x^2}\, dx$ on $[-2, 2]$. With such normalization, the joint eigenvalue density of GOE_n, GUE_n, GSE_n is proportional to

$$\prod_{\substack{j,k=1 \\ j<k}}^{n} |\lambda_j - \lambda_k|^\beta \prod_{j=1}^{n} e^{-\frac{\beta n}{4}\lambda_j^2} d\lambda_j, \tag{3.1}$$

$(\beta = 1, 2, 4$, respectively).

Now let us state the main result of the paper. Recall that by "eigenvalues" and "resonances" we call the zeros of the polynomial L^* in $\mathbb{C} \setminus \overline{\mathbb{D}}$ and $\overline{\mathbb{D}} \setminus \{0\}$, respectively, see the discussion in Sect. 2.1.

Theorem 3.1. *Let $\widetilde{\mathcal{H}}$ be given by* (1.1) *where $\mathcal{H}$ is from GOE_n, GUE_n or GSE_n; $\gamma \neq 0$ is a given constant; and κ is a random variable distributed on $(0, \infty)$ according to $F(\kappa)d\kappa$, independently of $\mathcal{H}$. Then resonances and eigenvalues $\{z_j\}_{j=1}^{2n}$*

of $\widetilde{\mathcal{H}}$ are jointly distributed on the set $S(2n)$ according to

$$\frac{1}{d_{2n,\beta}}\prod_{\substack{j,k=1\\j<k}}^{2n}|z_j-z_k|\prod_{\substack{j,k=1\\j<k}}^{2n}|1-z_j\bar{z}_k|^{\frac{\beta}{2}-2}\prod_{j=1}^{2n}e^{-\frac{\beta n}{4\gamma^2}z_j^2}\left|\frac{1-|z_j|^2}{1-z_j^2}\right|^{\frac{\beta}{4}-2}$$
$$\times\, e^{\frac{\beta n\kappa^2}{2\gamma^2}}\frac{F(\kappa)}{\kappa^{\beta n-1}}\left|\bigwedge_{j=1}^{2n}dz_j\right|, \tag{3.2}$$

where $\kappa=\sqrt{1-\prod_{j=1}^{2n}z_j}$ and

$$d_{2n,\beta}=\pi^{n/2}2^{n/2+1}e^{\frac{\beta n^2}{2\gamma^2}}\left(\frac{2\gamma^2}{\beta n}\right)^{\frac{n}{2}+\frac{\beta n(n-1)}{4}}\prod_{j=1}^{n-1}\Gamma(\tfrac{\beta j}{2}).$$

Remarks. 1. The wedge notation we use above is defined as follows. Let $\{z_j\}_{j=1}^m$ (in the theorem above, $m=2n$) be a random point process that consists of M complex-conjugate (non-real) points and L real points. M and L are random but satisfy $0\le M\le\lfloor\frac{m}{2}\rfloor$, $0\le L\le m$, $L+2M=m$. Then for functions $f:\mathbb{C}^m\to\mathbb{C}$ invariant under permutation of its variables, we define

$$\int_X f(z_1,\dots,z_m)\left|\bigwedge_{j=1}^m dz_j\right| := \sum_{M=0}^{\lfloor\frac{m}{2}\rfloor}2^M\frac{1}{M!L!2^M}$$
$$\times\int_{X\cap X_{L,M}} f(x_1+iy_1,x_1-iy_1,\dots,x_M+iy_M,x_M-iy_M,r_1,\dots,r_L)$$
$$\times\, dx_1dy_1\cdots dx_Mdy_M\,dr_1\cdots dr_L, \tag{3.3}$$

where

$$X_{L,M}=\{(x_1+iy_1,x_1-iy_1,\dots,x_M+iy_M,x_M-iy_M,r_1,\dots,r_L)\in X:$$
$$x_j+iy_j\in\mathbb{C}\setminus\mathbb{R}\text{ for }1\le j\le M; r_j\in\mathbb{R}\text{ for }1\le j\le L\}.$$

Note that 2^M here comes from $|d(x+iy)\wedge d(x-iy)|=2\,dx\,dy$ and $M!L!2^M$ comes from counting vectors in $X_{L,M}$ that represent the same configuration $\{z_j\}_{j=1}^m$. See [1, Sect. 2–3] for a more careful and rigorous discussion of these types of measures.

2. When κ is deterministic and equal to 1, then there are $2n-1$ resonances/eigenvalues. They belong to $S(2n-1)$ and following the same arguments as in the proof below, one can show that their joint distribution is

$$\frac{1}{d_{2n-1,\beta}}\prod_{\substack{j,k=1\\j<k}}^{2n-1}|z_j-z_k|\prod_{\substack{j,k=1\\j<k}}^{2n-1}|1-z_j\bar{z}_k|^{\frac{\beta}{2}-2}\prod_{j=1}^{2n-1}e^{-\frac{\beta n}{4\gamma^2}z_j^2}\left|\frac{1-|z_j|^2}{1-z_j^2}\right|^{\frac{\beta}{4}-2}\left|\bigwedge_{j=1}^{2n}dz_j\right|, \tag{3.4}$$

where

$$d_{2n-1,\beta} = \pi^{n/2} 2^{n/2} e^{\frac{\beta n(n-1)}{2\gamma^2}} \left(\frac{2\gamma^2}{\beta n}\right)^{\frac{n}{2}+\frac{\beta n(n-1)}{4}} \prod_{j=1}^{n-1} \Gamma(\tfrac{\beta j}{2}).$$

3. One can also work out the case when κ is deterministic but not 1. Note that in that case the eigenvalues/resonances belong to the subset of $S(2n)$ given by $\prod_{j=1}^{2n} z_j = 1 - \kappa^2$ (see Lemma 2.1(i)). See [18] for an analogue of this for non-Hermitian perturbations of finite matrices.

4. Compare (3.2) and (3.4) with (3.1). Their zeros are precisely the resonances/eigenvalues of $\widetilde{\mathcal{H}}$ and eigenvalues of $\mathcal{H}$ (after the inverse of $z + z^{-1}$ map — see (2.3)), respectively. Observe the following heuristics for the intuition. If the coupling κ is small, then by (2.4), L_{2n}^* is a small perturbation of K_{2n}. Therefore each eigenvalue of $\gamma\mathcal{H}$ on $(-2,2)$ will produce two complex-conjugate zeros of K_{2n} on $\partial\mathbb{D} \setminus \{\pm 1\}$, and so (see Sect. 2.3) two complex-conjugate zeros of L_{2n}^* (resonances of $\widetilde{\mathcal{H}}$) in $\mathbb{D}\setminus\mathbb{R}$ (provided κ is sufficiently small). Similarly, each eigenvalue of $\gamma\mathcal{H}$ on $\mathbb{R}\setminus[-2,2]$ will produce two real zeros of K_{2n}, one in $\mathbb{D}\cap\mathbb{R}$ and one in $\mathbb{R}\setminus\overline{\mathbb{D}}$, and so two real zeros of L_{2n}^*, also one in $\mathbb{D}\cap\mathbb{R}$ and one in $\mathbb{R}\setminus\overline{\mathbb{D}}$ (i.e., one eigenvalue and one resonance of $\widetilde{\mathcal{H}}$). In particular, if all the zeros of $\gamma\mathcal{H}$ are concentrated in $(-2,2)$, then $\widetilde{\mathcal{H}}$ will have only resonances without eigenvalues, provided κ is small.

5. When H is from the GUE_n ensemble, i.e., when $\beta = 2$, then the distribution (3.2) simplifies to

$$\frac{1}{d_{2n,2}} \prod_{\substack{j,k=1 \\ j<k}}^{2n} |z_j - z_k| \prod_{j=1}^{2n} e^{-\frac{n}{2\gamma^2} z_j^2} \left(e^{\frac{n\kappa^2}{\gamma^2}} \frac{F(\kappa)}{\kappa^{2n-1}} \right) \left| \bigwedge_{j=1}^{2n} dz_j \right|.$$

Similarly for (3.4).

Proof. Every $n \times n$ matrix can be tridiagonalized via the repeated application of the Householder transformations. Applying this to a random matrix $\mathcal{H}_n$ taken from one of the GOE_n, GUE_n, GSE_n ensembles, Dumitriu–Edelman showed that there exists a unitary matrix U_n such that

$$\mathcal{J}_n = U_n^* \mathcal{H}_n U_n = \begin{pmatrix} s_1 & t_1 & 0 & & \\ t_1 & s_2 & t_2 & \ddots & \\ 0 & t_2 & s_3 & \ddots & 0 \\ & \ddots & \ddots & \ddots & t_{n-1} \\ & & 0 & t_{n-1} & s_n \end{pmatrix}. \tag{3.5}$$

Moreover, U_n is independent of $\mathcal{J}_n$, satisfies

$$U_n \mathbf{e}_1 = U_n^* \mathbf{e}_1 = \mathbf{e}_1, \tag{3.6}$$

and the joint distribution of the coefficients $\{s_j\}_{j=1}^n$ and $\{t_j\}_{j=1}^{n-1}$ is

$$\frac{1}{c_{n,\beta}} \prod_{j=1}^{n-1} t_j^{\beta(n-j)-1} e^{-\beta n t_j^2/2}\, dt_j \prod_{j=1}^{n} e^{-\beta n s_j^2/4}\, ds_j, \tag{3.7}$$

where

$$c_{n,\beta} = \frac{\pi^{n/2}}{2^{n/2-1}} \left(\frac{2}{\beta n}\right)^{\frac{n}{2}+\frac{\beta n(n-1)}{4}} \prod_{j=1}^{n-1} \Gamma(\tfrac{\beta j}{2}) \tag{3.8}$$

(this follows from Dumitriu–Edelmam [4] after rescaling). Here $\beta = 1, 2, 4$ for GOE_n, GUE_n, GSE_n, respectively. In fact, for any $0 < \beta < \infty$, $\mathcal{J}_n$ in (3.5) with (3.7), (3.8) is a well-defined random matrix, whose eigenvalue distribution is (proportional to) (3.1).

Now let $\widetilde{\mathcal{H}}$ be given by (1.1) where $\mathcal{H} = \mathcal{H}_n$ is from GOE_n, GUE_n or GSE_n; $\gamma \neq 0$ is a given constant; and κ is a random variable distributed on $(0, \infty)$ and independent from $\mathcal{H}$. Let R be an $n \times n$ matrix with 1's on the anti-diagonal and 0's everywhere else. By the invariance of the Gaussian ensembles, $R^*\mathcal{H}_n R^*$ belongs to the same random matrix ensemble as $\mathcal{H}_n$. Now define U_n as above but applied to random matrix $R^*\mathcal{H}_n R$ instead of $\mathcal{H}_n$. Then $U_n^* R^* \mathcal{H}_n R U_n = \mathcal{J}_n$ and (3.6) holds. Define $\widetilde{U} = (R^* U_n R) \oplus I$ on $\ell^2(\mathbb{Z}_+)$. Then (3.6) implies $RU_nR^*\mathbf{e}_n = RU_n^*R^*\mathbf{e}_n = \mathbf{e}_n$, so that we get

$$\widetilde{U}^*\widetilde{\mathcal{H}}\widetilde{U} = \left(\begin{array}{c|ccc} \gamma R\mathcal{J}_n R^* & \kappa & & \\ \hline \kappa & 0 & 1 & \\ & 1 & 0 & \ddots \\ & & \ddots & \ddots \end{array}\right).$$

This means that $\widetilde{H}$ is unitarily equivalent to a Jacobi operator $\mathcal{J}(\mathbf{a}, \mathbf{b})$ (see (2.1)) with $\mathbf{a} = \{\gamma t_{n-1}, \gamma t_{n-2}, \ldots, \gamma t_1, \kappa, 1, 1, \ldots\}$ and $\mathbf{b} = \{\gamma s_n, \gamma s_{n-1}, \ldots, \gamma s_1, 0, 0, \ldots\}$ (in other words, the Dumitriu–Edelman coefficients are order-reversed, scaled by γ and then coupled to the free Jacobi operator with coupling κ).

As stated in Sect. 2.3, there is a one-to-one correspondence between the $2n$ Jacobi coefficients $\mathbf{a}, \mathbf{b} \in \mathbb{R}_+^n \times \mathbb{R}^n$ and $2n$ zeros in $S(2n)$ of the (reversed) perturbation determinant L_{2n}^*. We will compute the Jacobian of this transformation by computing one step at a time:

Lemma 3.2. *Let*

$$L_j^*(z) = z^j + u_{j-1}^{(j)} z^{j-1} + u_{j-2}^{(j)} z^{j-2} + \cdots + u_1^{(j)} z + u_0^{(j)}.$$

Then (2.4) *and* (2.5) *imply*

$$\det \frac{\partial\left(u_{2k}^{(2k+1)}, u_{2k-1}^{(2k+1)}, \dots, u_0^{(2k+1)}\right)}{\partial\left(u_{2k-1}^{(2k)}, u_{2k-2}^{(2k)}, \dots, u_0^{(2k)}, b_{k+1}\right)} = -1 \tag{3.9}$$

and

$$\det \frac{\partial\left(u_{2k+1}^{(2k+2)}, u_{2k}^{(2k+2)}, \dots, u_0^{(2k+2)}\right)}{\partial\left(u_{2k}^{(2k+1)}, u_{2k-1}^{(2k+1)}, \dots, u_0^{(2k+1)}, a_{k+1}\right)} = -2a_{k+1}^{2k+1}. \tag{3.10}$$

Proof. Let $K_{2k}(z) = K_{2k+1}(z) = z^{2k} + c_{2k-1}z^{2k-1} + \dots + c_1 z + 1$. We will also put $c_{2k} = c_0 = 1$ and $c_j = 0$ for $j < 0$ or $j > 2k$. Note that $c_j = c_{2k-j}$ for all j since $K_{2k} = K_{2k}^*$.

Equality (2.7) implies that for each $j \le k$, $c_j - c_{j-2} = u_{2k-j}^{(2k)} - u_{j-2}^{(2k)}$, which shows that c_j (for $j \le k$) does not depend on the coefficients $u_l^{(2k)}$ with $j - 1 \le l \le 2k - j - 1$.

Now, (2.5) implies $u_j^{(2k+1)} = u_{j-1}^{(2k)} - b_{k+1}c_j$. Using this, we can show that the Jacobian matrix

$$\frac{\partial\left(u_0^{(2k+1)}, u_{2k}^{(2k+1)}, u_1^{(2k+1)}, u_{2k-1}^{(2k+1)}, \dots, u_{k-1}^{(2k+1)}, u_{k+1}^{(2k+1)}, u_k^{(2k+1)}\right)}{\partial\left(b_{k+1}, u_{2k-1}^{(2k)}, u_0^{(2k)}, u_{2k-2}^{(2k)}, \dots, u_{k-2}^{(2k)}, u_k^{(2k)}, u_{k-1}^{(2k)}\right)} \tag{3.11}$$

has a triangular structure. Indeed, $u_0^{(2k+1)} = -b_{k+1}$, $u_{2k}^{(2k+1)} = u_{2k-1}^{(2k)} - b_{k+1}$. Furthermore, $u_1^{(2k+1)} = u_0^{(2k)} - b_{k+1}c_1$, $u_{2k-1}^{(2k+1)} = u_{2k-2}^{(2k)} - b_{k+1}c_1$; and as we saw earlier c_1 is a independent of $u_l^{(2k)}$ with $0 \le l \le 2k-2$. This can be continued by induction. The determinant of the triangular matrix (3.11) is equal to the product of the diagonal entries, which equals to -1. This proves (3.9).

Similar arguments prove (3.10), with just one extra wrinkle. Equality (2.8) shows that for each $j \le k$, $c_j - c_{j-2} = u_{2k-j+1}^{(2k+1)} - u_{j-1}^{(2k+1)}$, which shows that c_j (for $j \le k$) is equal to $-u_{j-1}^{(2k+1)} + d_j$, where d_j does not depend on the coefficients $u_l^{(2k+1)}$ with $j - 1 \le l \le 2k - j$. Then we show that the Jacobian matrix

$$\frac{\partial\left(u_{2k+1}^{(2k+2)}, u_0^{(2k+2)}, u_{2k}^{(2k+2)}, \dots, u_{k-1}^{(2k+2)}, u_{k+1}^{(2k+2)}, u_k^{(2k+2)}\right)}{\partial\left(u_{2k}^{(2k+1)}, a_{k+1}, u_{2k-1}^{(2k+1)}, u_0^{(2k+1)}, \dots, u_{k-2}^{(2k+1)}, u_k^{(2k+1)}, u_{k-1}^{(2k+1)}\right)} \tag{3.12}$$

has a triangular structure. Indeed, using (2.4), we get $u_j^{(2k+2)} = u_{j-1}^{(2k+1)} + (1 - a_{k+1}^2)c_j$. This implies $u_{2k+1}^{(2k+2)} = u_{2k}^{(2k+1)}$; $u_0^{(2k+2)} = 1 - a_{k+1}^2$, $u_{2k}^{(2k+2)} = u_{2k-1}^{(2k+1)} + (1 - a_{k+1}^2)$. Furthermore, $u_1^{(2k+2)} = u_0^{(2k+1)} + (1 - a_{k+1}^2)c_1 = a_{k+1}^2 u_0^{(2k+1)} + (1 - a_{k+1}^2)d_1$; $u_{2k-1}^{(2k+2)} = u_{2k-2}^{(2k+1)} + (1 - a_{k+1}^2)c_1$; and as we saw earlier d_1 depends only on $u_{2k}^{(2k+1)}$, while c_1 depends only on $u_{2k}^{(2k+1)}$ and $u_0^{(2k+1)}$. This together with an induction shows the triangular structure. The determinant of (3.12) is then equal to the product of the diagonal entries, which equals to $1 \times (-2a_{k+1}) \times 1 \times (a_{k+1}^2)^k$. This proves (3.10). ☐

Now we are ready to compute the main Jacobian.

Lemma 3.3. *Let* $\{a_j, b_j\}_{j=1}^n \in \mathbb{R}_+^n \times \mathbb{R}^n$ *be the first Jacobi coefficients of* $\mathcal{J}$*, and let* $\{z_j\}_{j=1}^{2n} \in S(2n)$ *be the zeros of* L_{2n}^**. Then the following change of variables holds true:*

$$\prod_{j=1}^n da_j\, db_j = \frac{\prod_{j<k} |z_j - z_k|}{2^n \prod_{j=1}^n a_j^{2j-1}} \left| \bigwedge_{j=1}^{2n} dz_j \right|. \tag{3.13}$$

Proof. Applying the previous lemma recursively, we obtain

$$\det \frac{\partial \left(u_{2n-1}^{(2n)}, u_{2n-2}^{(2n)}, \dots u_0^{(2n)} \right)}{\partial \left(b_1, a_1 \dots, b_{k-1}, a_{k-1}, b_k, a_k \right)} = 2^n \prod_{j=1}^n a_j^{2j-1}.$$

Finally, the change of variables

$$\prod_{j=0}^{2n-1} du_j^{(2n)} = \prod_{j<k} |z_j - z_k| \left| \bigwedge_{j=1}^{2n} dz_j \right|$$

follows from the arguments in [14, Lemma 6.5] (we warn the reader of the missing factor $1/(M!L!2^M)$ that is needed in [14, Eq. (3.3)]). Combining the last two formulas, we obtain (3.13). ☐

Now recall that we are computing zeros of L_{2n}^* for the Jacobi matrix $\mathcal{J}(\mathbf{a}, \mathbf{b})$ with $\mathbf{a} = \{\gamma t_{n-1}, \gamma t_{n-2}, \dots, \gamma t_1, \kappa, 1, 1, \dots\}$ and $\mathbf{b} = \{\gamma s_n, \gamma s_{n-1}, \dots, \gamma s_1, 0, 0, \dots\}$, where the distribution of $\{t_j, s_j\}$ is given in (3.7). Performing the order-reversal and scaling, we obtain that the joint distribution of $\{a_j, b_j\}_{j=1}^n$ is

$$\frac{1}{\widetilde{c}_{n,\beta}} \prod_{j=1}^{n-1} a_j^{\beta j - 1} e^{-\beta n a_j^2/(2\gamma^2)}\, da_j \prod_{j=1}^n e^{-\beta n b_j^2/(4\gamma^2)}\, db_j F(a_n)\, da_n,$$

where

$$\widetilde{c}_{n,\beta} = \frac{\pi^{n/2}}{2^{n/2-1}} \left(\frac{2\gamma^2}{\beta n} \right)^{\frac{n}{2} + \frac{\beta n(n-1)}{4}} \prod_{j=1}^{n-1} \Gamma(\tfrac{\beta j}{2}).$$

Applying Lemma 3.3, we obtain that this is equal to

$$\frac{1}{2^n \widetilde{c}_{n,\beta}} \prod_{j=1}^{n-1} a_j^{(\beta-2)j} e^{-\beta n a_j^2/(2\gamma^2)} \prod_{j=1}^n e^{-\beta n b_j^2/(4\gamma^2)} \frac{F(a_n)}{a_n^{2n-1}} \prod_{j<k} |z_j - z_k| \left| \bigwedge_{j=1}^{2n} dz_j \right|.$$

Now applying parts (i), (iv), and (v) of Lemma 2.1 easily leads to the distribution (3.2). ☐

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Modern results in the spectral analysis for a class of integral-difference operators and application to physical processes

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Devoted to the memory of Prof. B.S. Pavlov

Abstract. The review of the results obtained in the spectral analysis for a class of integral-difference operators and their application to physical processes, obtained since late 1990s until now, is provided. Some fresh not yet published results in the field are also presented. We demonstrate the physical background and the logical structure of the corresponding studies. The discussion includes both the 1D case and the recent generalization to higher dimensions. We trace the links with different fields of mathematics. In particular, a new class of special functions that naturally appear as the kernels of the mentioned operators, is discussed. The open problems are highlighted and further possible encouraging investigations are proposed.

Keywords. Integral-difference operators; spectral estimations; special functions; inverse problems.

1. Introduction and physical background

In the present paper we provide a summary of the results in the spectral analysis for a class of integral-difference operators $\mathcal{K}_\varphi$ defined as

$$\mathcal{K}_\varphi : u(\mathbf{x}) \mapsto \int_{\mathbb{R}^M} \frac{u(\mathbf{x})\varphi(\mathbf{s}) - u(\mathbf{s})\varphi(\mathbf{x})}{|\mathbf{x}-\mathbf{s}|}\, d^M\mathbf{s} \tag{1}$$

on the Hilbert space $L_2(\mathbb{R}^M)$. Operator $\mathcal{K}_\varphi$ is the Friedrichs extension [1, 2] of the core operator defined in a domain $\mathcal{D} = C^1(\mathbb{R}^M) \cap L_1(\mathbb{R}^M) \cap L_2(\mathbb{R}^M)$. Function $\varphi(\mathbf{x})$ is the functional parameter, which properties and the physical meaning are discussed below.

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Originally, the operators $\mathcal{K}_\varphi$ in the 1D case $M = 1$ were introduced as collision operators [3] in a non-equilibrium statistical physics [4, 5] model of 1D gas. In this model the functional parameter $\varphi(\mathbf{x}) \geq 0$ plays the role of the equilibrium distribution. The discrete spectrum of the operator $\mathcal{K}_\varphi$ generates the Lyapunov exponentials, determining the rates with which the system goes to the equilibrium state [4]. Physicists have been interested in the dynamics of the relaxation of the system to equilibrium determined by the equilibrium distribution function $\varphi(x)$. There were introduced functions $U(x,t)$ considered as the probability densities for a 1D gas. In the first order approximation, the relaxation process is described by the following dynamical equation:

$$\frac{\partial}{\partial t} U(x,t) = -\,\mathcal{K}_\varphi\, U(x,t) \tag{2}$$

Thus, the spectrum $\sigma(\mathcal{K}_\varphi)$ of the operator $\mathcal{K}_\varphi$ determines the relaxation speeds of the different modes. In particular, for the discrete modes $\tau_n^\varphi \in \sigma_d(\mathcal{K}_\varphi)$, $\mathcal{K}_\varphi u_n^\varphi = \tau_n^\varphi u_n^\varphi$,

$$U(x,t) = \sum_n u_n^\varphi(x)\, e^{-\tau_n^\varphi\, t}\,, \quad \text{where}\, U(x,0) = \sum_n u_n^\varphi(x)\,.$$

and τ_n^φ are the Lyapunov coefficients of relaxation [4, 5, 3] (the eigenvalues of the operator $\mathcal{K}_\varphi$).

However, the empiric approach to the spectral analysis of the corresponding operators [3] did not allow for the trustworthy results, which demanded the rigorous mathematical study. Such study started in late 1990s [6] and has been continued in the next years [7]–[10]. The review of the first group of the results can be find in [10]. By 2004 further success of these studies was temporary blocked by the absence of the clear ways to weaken the demands to the functional parameter $\varphi(\mathbf{x})$ and to extend the investigation to the higher dimensions $M \geq 2$. Later some results on analytical solution of an integro-differential equation arising from a collision operator were obtained in [11]. At the same time the traced interesting links of the problem under investigation with various fields of mathematics remained an encouraging factor for the continuation of the studies. The details are provided below in Section 3 of the present paper.

Other encouraging factors have come from the interest of physicists. Similar problems appeared for different physical systems and processes. They include processes in nanostructures due to the necessity to model electrolyte relaxation in thin films [12]. Application of operators $\mathcal{K}_\varphi$ in the 2D and 3D spaces to the dynamics of the matter relaxation processes in the external attractive fields $\varphi(\mathbf{x}) \geq 0$ was developed. [13]. Namely, in the proposed model the dynamics of the matter density $U(\mathbf{x},t)$ is determined by the field $\varphi(\mathbf{x})$ in the following way. There are two competing processes $\mathbf{P}_+$ and $\mathbf{P}_-$. In a vicinity of a point $\mathbf{x} \in \mathbb{R}^M$ during the time interval δt the portion of the matter (attracted by the field $\varphi(x)$) is increased by incoming portions from vicinities of all points $\mathbf{s} \in \mathbb{R}^M$. If the speed of interaction is homogeneous, the overall increase of the matter density $U(\mathbf{x},t)$ in point $\mathbf{x}$ during the time interval δt due to the process $\mathbf{P}_+$ is

$$(\mathbf{P}_+) \qquad \delta U_+(\mathbf{x},t) = \delta t\, \varphi(\mathbf{x}) \int_{\mathbb{R}^M} \frac{U(\mathbf{s},t)}{|\mathbf{x}-\mathbf{s}|}\, d^M\mathbf{s}\,.$$

Similarly, the inverse process (moving of the matter from a vicinity of point $\mathbf{x}$ to vicinities of all other points $\mathbf{s} \in \mathbb{R}^M$ is described by

$$(\mathbf{P}_-) \qquad \delta U_-(\mathbf{x},t) = -\,\delta t\, U(\mathbf{x},t) \int_{\mathbb{R}^M} \frac{\varphi(\mathbf{s})}{|\mathbf{x}-\mathbf{s}|}\, d^M\mathbf{s}\,.$$

Combining these two processes $\mathbf{P}_+$ and $\mathbf{P}_-$ and taking the limit $\delta t \to 0$ we get the dynamical equation

$$\frac{\partial}{\partial t} U(\mathbf{x},t) = -\,\mathcal{K}_\varphi\, U(\mathbf{x},t) \tag{3}$$

similar to Eq. (2), but for $\mathbb{R}^M$ of any dimension M. Let us note, that if $\mathcal{K}_\varphi$ are treated as the operators underlying the processes of the matter relaxation in the attractive field $\varphi(\mathbf{x})$ and the functions $U(\mathbf{x},t)$ are considered to be the matter densities, the matter could be either an ionised gas, or a liquid containing charged particles (in this case $U(\mathbf{x},t)$ is the density of charged particles in electrolyte). For dimension $M = 1$, the corresponding system may be a thin tube, where the field is parallel to the tube axis. For dimension $M = 2$, the system may be a monomolecular layer of electrolyte on a surface. Alternatively, in 2-dimensional case $U(\mathbf{x},t)$ can be treated as the thickness of the electrolyte layer on a surface. In dimension $M = 3$, the physical interpretation is obvious. Higher dimensions $M \geq 4$ may appear in some service structures for certain systems. Of course, some modifications may be needed for practical applications to specific physical systems.

The corresponding spectral estimates were obtained for specific fields [14, 15]. The necessary generalization of the developed technique to the higher-dimensional spaces $M \geq 2$ became possible due to the quadratic forms approach [1, 2] explored for the problems under investigation in [13]. The details are provided below in Sect. 4 of the present paper.

Similar spectral problems appear also in the models of several physical processes. Carrier scattering in metals and semiconductors was considered in [16]. It elucidates the state of the art in the research on the scattering mechanisms for current carriers in metals and semiconductors and describes experiments in which these mechanisms are most dramatically manifested. The subjects dealt with include: electronic transport theory based on the test-particle and correlation-function concepts; scattering by phonons, impurities, surfaces, magnons, dislocations, electron-electron scattering and electron temperature; two-phonon scattering, spin-flip scattering, scattering in degenerate and many-band models.

In [17] the subband structure in a smooth film where isotropic volume scattering gives rise to a finite mean free path was studied. The intersubband transitions into both the propagating and evanescent modes were described by an infinite system of equations. Its solution determines self-consistently the scattering-induced level broadening. The thickness dependence of the density of states and the conductivity are discussed in detail and compared with results which follow from the neglect of level broadening. For typical mean free paths, level broadening strongly smears out the steps of the density of states and suppresses size-induced oscillations of the conductivity.

In [18] the additional resistivity of a quantum film due to an obstacle was investigated. The film was treated by a semi-classical formalism whilst the obstacle is characterized by its quantum mechanical scattering cross-section. The film intrinsic scattering mechanism allows for the adaptation of an arbitrary density distribution to a characteristic “ideal” distribution over the channels. Special attention was paid to the multiple-scattering cycles between the obstacle and its surroundings, i.e., the scattering background of the film. The analysis of these backscattering processes has lead to a self-consistent equation for the current density incident on the scatterer. For the general case of an arbitrarily strong obstacle and many conducting channels, this equation system can be solved only numerically. However, the formalism becomes handy if the obstacle scatters only weakly. A condition is found for the obstacle to be considered as weak. On the other hand, if one considers only one conducting channel it is possible to solve the transport problem analytically even for a strong obstacle.

In [19] the problem of the residual resistivity dipole (formulated by Landauer in 1957, see, e.g., [20]) was reconsidered for a spherically symmetric obstacle which is small compared to the bulk mean free path but otherwise arbitrary. A classical formalism was developed which rests on a local kinetic equation. The current density incident on the obstacle is the central quantity that allowed to calculate all relevant quantities.

In [21] the extra resistivity due to a planar perturbation in an otherwise homogeneous bulk medium was considered. The current density incident on the barrier and the density distribution in the bulk were calculated self-consistently as a solution of a classical diffusion problem. Numerical calculations have shown fluctuations of the density within a few bulk mean free paths in the vicinity of the barrier. They depend sensitively on the transmission and reflection coefficients. The occurrence of the density fluctuations generally prevents the derivation of a simple generalization of the one-dimensional Landauer formula. Instead, a more involved expression for the extra resistivity was found in a simplified model of discrete angles of carrier motion.

In [22], similar to the Landauer–Büttiker approach to transport [23], a resistor was characterized by its reflection and transmission coefficients. Such a transmitter is coupled incoherently to two resistive quantum wires. These leads define an asymptotic current-distribution over the different channels and allowed to adapt the current distribution to the transmitter. For carriers at fixed energy, the resistance was defined via asymptotic density differences of the diffusing carriers. This resistance, and the corresponding current distribution, were found by minimizing a variational functional that is additively composed of lead and transmitter terms.

The resistance functional was defined for the transmitter alone, coupled incoherently to leads with unspecified properties, especially to ideal leads and reservoirs. The said functional is additive for transmitters in series if interference effects between them are excluded. The contacts between ideal leads and reservoirs can be modeled as special transmitters, reproducing thus the standard results for the total resistance.

In [24] for a non-interacting quantum-particle gas in a near-equilibrium steady state a general expression for the entropy production was given. The particles are scattered by a cluster of scatterers that are coupled incoherently via connecting ideal leads. The internal current and/or density distribution were determined by minimizing the entropy production. This quantity is invariant under a transformation where differences in particle density are replaced by those in electrostatic potential.

In [23] electronic transport in mesoscopic systems has been considered.

The historically formed logical structure of the investigations in the field under consideration is the following. The consideration of various physical systems [3], [12]–[19], [21, 22, 24] has led to the dynamical equations referring to the operators similar to $\mathcal{K}_\varphi$. As the empiric approach to the spectral analysis sometimes fails (e.g., for the model of non-equilibrium 1D gas [3]), the development of the rigorous mathematical approach has been required. Such approach has been developed in [6] - [15] later on. The review of the results in the 1D case can be find in [10]. Next, the application of the quadratic form approach has allowed for the generalization to the higher dimensions [13] and the investigation of matter relaxation processes in attractive fields for specific 2D [14] and 3D [15] systems.

The problems under investigation have demanded the exploitation of the techniques coming from numerous fields of mathematics, like various methods of the linear operator analysis [1, 2], including the quadratic form approach; asymptotic analysis [27]; theory of orthogonal polynomials and special functions [31]–[40]. Links with other fields of mathematics, like Jacobi matrices with unbounded entries [25, 26] and weighted mean-square deviation functionals have also been traced [13]. The discussed investigation have contributed to these fields through side results, like a new property of the Legendre polynomials [13]. In particular, it was shown that the operators $\mathcal{K}_\varphi$ under consideration in the higher-dimensional cases $\mathbf{x} \in \mathbb{R}^M$, $M \geq 2$ naturally generates a new class of special functions $\Xi_N^{[\mathbf{k}]}$, $N = M - 1 = 1, 2, 3, \ldots$; $\mathbf{k} \in \mathbb{Z}^N$. These functions were introduced in [13] and investigated in [14] for $N = 1$ and in [15] for $N = 2$ (see also Sect. 5 of the present paper).

The present paper is organized as follows. In Sect. 2 we give the necessary definitions and discuss the general spectral structure of the operators $\mathcal{K}_\varphi$. Sections 3 and 4 are devoted to the detailed results in the spectral analysis of these operators in dimensions $M = 1$ and $M \geq 2$ correspondingly. Section 5 provides the results for the class of special functions generated by the operators $\mathcal{K}_\varphi$ for $M \geq 2$. In Sect. 6 the links with other fields of mathematics are traced. In Sect. 7

we consider the inverse problem for operators $\mathcal{K}_\varphi$ Finally, in Sect. 8 we summarize the modern results in the field and outline further tasks and open problems.

For previously published results we do not repeat in the present paper the technical proofs, but just highlight the key points and trace the general underlying methods used.

2. Acceptable functional parameters $\varphi(\mathbf{x})$ and the general spectral structure of the corresponding operators $\mathcal{K}_\varphi$

In order to be able using the resolvent comparison approach [6, 10] (see also Sect. 3 below) underlying the spectral analysis of the operator $\mathcal{K}_\varphi$ introduced in [6] and further discussed in [10] (for $M = 1$) and [13] (for $M \geq 2$), we restrict our consideration to the so called *acceptable functions* $\varphi(\mathbf{x})$.

Definition 1. *Function $\varphi(\mathbf{x})$ in $\mathbb{R}^M$ is called as acceptable function if it is non-negative, summable, of Lipshitz-1 class on its support and is uniformly separated from zero in its support* $\operatorname{supp}\varphi = \Omega \subset \mathbb{R}^M$. *Namely, this means that $\varphi(\mathbf{x})$ satisfies the following conditions:*

$$0 \leq \varphi(\mathbf{x}) \in L_1(\mathbb{R}^M)\,; \tag{4}$$

$$\exists\, A_\varphi \geq 0 :\ |\varphi(\mathbf{x}) - \varphi(\mathbf{s})| \leq A_\varphi\, |\mathbf{x} - \mathbf{s}|\,,\ \forall \mathbf{x}, \mathbf{s} \in \Omega = \operatorname{supp}\varphi\,; \tag{5}$$

$$\exists\, \varepsilon_\varphi > 0 :\ |\varphi(\mathbf{x})| \geq \varepsilon_\varphi\,,\ \forall\, \mathbf{x} \in \Omega\,. \tag{6}$$

Note, that the conditions (4) and (6) can be satisfied simultaneously only if the domain $\Omega \subset \mathbb{R}^M$ has a finite volume $\operatorname{Vol}(\Omega) < \infty$.

Later we will restrict our consideration to the so called *admissible domains* Ω. They are defined as follows.

Definition 2. *In 1D case ($M = 1$) the domain $\Omega \subset \mathbb{R}$ is called as admissible domain if it is a union of a countable set of finite intervals*

$$\Omega = \bigcup_j (a_j, b_j)$$

with finite total volume

$$V_\Omega := \operatorname{Vol}(\Omega) = \sum_j |b_j - a_j| < \infty\,.$$

Definition 3. *For higher dimensions ($M \geq 2$) the domain $\Omega \subset \mathbb{R}^M$ is called as admissible domain if it is a compact convex domain.*

In Sect. 4 below some more strong demands to the domain $\Omega \subset \mathbb{R}^M$ will be introduced in order to get specific results in spectral estimations for the corresponding operators $\mathcal{K}_\varphi$.

As mentioned above in Sect. 1, for the collision operators the function $\varphi(\mathbf{x})$ plays the role of the equilibrium distribution function [6, 7, 9, 10] and has the physical meaning of probability density. For the matter relaxation processes [13, 14, 15] the function $\varphi(\mathbf{x})$ plays the role of an external attractive field. This makes the conditions (4) and (5) very natural from the physical point of view. At the same time the requirement (6) originally appeared by mathematical reasons (as its violation in dimension 1 prevents obtaining important spectral estimations [10, 13]). However, it also has a physical background: if we consider a conductor with an induced field, generally, the field vanishes outside the body of the conductor (the remark by P. Avtonomov).

Let us note the following:

Remark 1. (Equilibrium spectral point)

From formula (1) it obviously follows that for any $\varphi(\mathbf{x}) \in \mathcal{D}$ point $\lambda = 0$ belongs to the spectrum of the operator $\mathcal{K}_\varphi$ and corresponds to the equilibrium function $u_0(\mathbf{x}) \equiv \varphi(\mathbf{x})$. Physically it means that the system in the state of the equilibrium does not evolve in time.

One can decompose the original Hilbert space $\mathcal{H} = L_2(\mathbb{R}^M)$ into orthogonal sum $\mathcal{H} = \mathcal{H}^{\mathrm{i}} \oplus \mathcal{H}^{\mathrm{e}}$, where we use the notations $\mathcal{H}^{\mathrm{i}} := L_2(\Omega)$ and $\mathcal{H}^{\mathrm{e}} := L_2(\mathbb{R}^M \backslash \Omega)$. This allows for the corresponding decomposition of the operator $\mathcal{K}_\varphi$, i.e., for its representation in the following matrix form [6, 7, 10, 13]:

$$\mathcal{K}_\varphi = \begin{pmatrix} \mathcal{K}_\varphi^{\mathrm{ii}} & \mathcal{K}_\varphi^{\mathrm{ie}} \\ \mathcal{K}_\varphi^{\mathrm{ei}} & \mathcal{K}_\varphi^{\mathrm{ee}} \end{pmatrix}, \tag{7}$$

where $\mathcal{K}_\varphi^{\mathrm{pq}} : \mathcal{H}^{\mathrm{q}} \to \mathcal{H}^{\mathrm{p}}$, i.e., in formula (1) $\mathbf{s} \in \Omega$ for q = i, $\mathbf{s} \in \mathbb{R}^M \backslash \Omega$ for q = e, $\mathbf{x} \in \Omega$ for p = i and $\mathbf{x} \in \mathbb{R}^M \backslash \Omega$ for p = e. Introducing the orthogonal projection operators $\mathcal{P}_{\mathrm{p}}$ on the subspaces $\mathcal{H}^{\mathrm{p}}$ in $\mathcal{H} = L_2(\mathbb{R}^M)$, one can write $\mathcal{K}_\varphi^{\mathrm{pq}} = \mathcal{P}_{\mathrm{p}} \mathcal{K}_\varphi \mathcal{P}_{\mathrm{q}}$. In the representation (7) the spectral problem

$$\mathcal{K}_\varphi u = \lambda u \tag{8}$$

turns into

$$\begin{pmatrix} \mathcal{K}_\varphi^{\mathrm{ii}} & \mathcal{K}_\varphi^{\mathrm{ie}} \\ \mathcal{K}_\varphi^{\mathrm{ei}} & \mathcal{K}_\varphi^{\mathrm{ee}} \end{pmatrix} \begin{pmatrix} u^{\mathrm{i}} \\ u^{\mathrm{e}} \end{pmatrix} = \lambda \begin{pmatrix} u^{\mathrm{i}} \\ u^{\mathrm{e}} \end{pmatrix}, \tag{9}$$

where $u^p := \mathcal{P}_{\mathrm{p}} u$, $\mathrm{p} \in \{\mathrm{i}, \mathrm{e}\}$.

Direct calculations [6, 10, 13] lead to the following results.

Lemma 1. *If $\varphi(\mathbf{x})$ is an acceptable function in the sense of Definition 1, then the operators $\mathcal{K}_\varphi^{\mathrm{pq}}$ in the representation (7) are*

$$\mathcal{K}_\varphi^{\mathrm{ii}} := K_\varphi : u(\mathbf{x}) \mapsto \int_\Omega \frac{u(\mathbf{x})\varphi(\mathbf{s}) - u(\mathbf{s})\varphi(\mathbf{x})}{|\mathbf{x} - \mathbf{s}|} \, d^M\mathbf{s}, \quad \mathbf{x} \in \Omega\,; \tag{10}$$

$$\mathcal{K}_\varphi^{\mathrm{ie}} : u(\mathbf{x}) \mapsto \int_{\mathbf{R}^M \backslash \Omega} \frac{u(\mathbf{s})}{|\mathbf{x} - \mathbf{s}|} \, d^M\mathbf{s}, \quad \mathbf{x} \in \Omega\,; \tag{11}$$

$$\mathcal{K}_\varphi^{\mathrm{ei}} \equiv 0\,; \tag{12}$$

$$\mathcal{K}_\varphi^{\mathrm{ee}} : u(\mathbf{x}) \mapsto q_\varphi(\mathbf{x})\, u(\mathbf{x}), \quad q_\varphi(\mathbf{x}) := \int_{\mathbb{R}^M \backslash \Omega} \frac{\varphi(\mathbf{s})}{|\mathbf{x} - \mathbf{s}|} \, d^M\mathbf{s}\,, \, \mathbf{x} \in \mathbf{R}^M \backslash \Omega\,. \tag{13}$$

Proof. of this lemma comes from simple straightforward calculations based on the expression (1). □

The operator K_φ defined by the expression (10) and acting in the Hilbert space $L_2(\Omega)$ is called as the *restricted operator*.

Remark 2. (Physical meaning of representation (7))

The restricted operator K_φ acts in the Hilbert space $L_2(\Omega)$ and would describe the dynamics of the system in Ω if the boundary $\partial\Omega$ is impenetrable. In higher dimensions $M \geq 2$ (see Sect. 4 below), being the sum of a compact integral operator and of an operator of the multiplication by the function $q_\varphi(\mathbf{x})$, it has a rich spectral structure. Its spectrum, as shown below, is non-negative. We are specially interested in its eigenvalues, which are the Lyapunov coefficients of relaxation of the corresponding modes. It was also shown [13] that the spectrum of the restricted operator K_φ is a subset of the spectrum of the original operator $\mathcal{K}_\varphi$. The operator $\mathcal{K}_\varphi^{\mathrm{ie}}$ describes mutual influence of the matter inside and outside any bounded convex domain Ω, while the operator q_φ is responsible for the "external" dynamics in $\mathbb{R}^M \backslash \Omega$. Equality (12), $\mathcal{K}_\varphi^{\mathrm{ei}} \equiv 0$, corresponds to physically clear fact of the absence of the matter flow from Ω (where the attractive field $\varphi(\mathbf{x}) \geq 0$) to $\mathbb{R}^M \backslash \Omega$ (where $\varphi(\mathbf{x}) \equiv 0$).

Lemma 1 allows for the general description of the spectrum of the operator $\mathcal{K}_\varphi$. Namely, the following statement is true.

Theorem 1. *If $\varphi(\mathbf{x})$ is an acceptable function in the sense of Definition 1, then the spectrum of the operator $\mathcal{K}_\varphi$ is the union of the spectra of restricted operator K_φ and the image of the function $q_\varphi(\mathbf{x})$, i.e.,*

$$\sigma(\mathcal{K}_\varphi) = \sigma(K_\varphi) \cup \mathcal{R}(q_\varphi) \,. \tag{14}$$

Proof. We follow the technique introduced in [6]. Decomposition $\mathcal{H} = \mathcal{H}^{\mathrm{i}} \oplus \mathcal{H}^{\mathrm{e}}$ allows for the representation of any function $u \in \mathcal{H}$ as the two-component function $u = (u^{\mathrm{i}}, u^{\mathrm{e}})^T$, where $u^{\mathrm{p}} \in \mathcal{H}^{\mathrm{p}}$. If the point $\lambda \in \sigma(K_\varphi)$ corresponds to the (generalized) eigenfunction u_λ^{i} of the restricted operator K_φ, we see that according to Lemma 1 $u_\lambda = (u^{\mathrm{i}}, u^{\mathrm{e}})^T$ is the (generalized) eigenfunction of the operator $\mathcal{K}_\varphi$ corresponding to the spectral point λ. Therefore, $\sigma(K_\varphi) \subset \sigma(\mathcal{K}_\varphi)$.

On the other hand, if $\lambda \in \mathcal{R}(q_\varphi)$ the delta-function(s) $\delta(\mathbf{x} - \mathbf{x}_\lambda)$ are the generalized eigenfunction(s) of the operator $\mathcal{K}_\varphi^{\mathrm{ee}}$ given by formula (13) if $\mathbf{x}_\lambda$ are the inverse images of the function $q_\varphi(\mathbf{x})$ in the point λ, i.e., $q_\varphi(\mathbf{x}_\lambda) = \lambda$. We take $u^{\mathrm{e}}(\mathbf{x}) = \delta(\mathbf{x} - \mathbf{x}_\lambda)$. If $\lambda \notin \sigma(K_\varphi)$, there exists the inverse operator $(K_\varphi - \lambda)^{-1}$. Due to the representation (7) we see that $\big((K_\varphi - \lambda)^{-1}[|\mathbf{x} - \mathbf{x}_\lambda|^{-1}] \,,\, \delta(\mathbf{x} - \mathbf{x}_\lambda)\big)^T$ are the generalized eigenfunction of the operator $\mathcal{K}_\varphi$ corresponding to the spectral point $\lambda \in \mathcal{R}(q_\varphi) \backslash \sigma(K_\varphi)$. Therefore, $\mathcal{R}(q_\varphi) \backslash \sigma(K_\varphi) \subset \sigma(\mathcal{K}_\varphi)$. Hence $\sigma(K_\varphi) \cup \mathcal{R}(q_\varphi) \subseteq \sigma(\mathcal{K}_\varphi)$.

Now let us assume that $\lambda \notin \sigma(K_\varphi) \cup \mathcal{R}(q_\varphi)$. As $\lambda \notin \mathcal{R}(q_\varphi)$, the component $u_\lambda^{\mathrm{e}} = \mathcal{P}_e u_\lambda$ of the corespondent solution u_λ of the spectral problem (8) is trivial, $u_\lambda^{\mathrm{e}}(\mathbf{x}) \equiv 0$. Then due to Lemma 1, $K_\varphi u_\lambda^{\mathrm{i}} = \lambda u_\lambda^{\mathrm{i}}$. As $\lambda \notin \sigma(K_\varphi)$ it means that

$u^{\mathrm{i}}_\lambda(\mathbf{x}) \equiv 0$. Thus $u_\lambda(\mathbf{x}) \equiv 0$, so $\lambda \notin \sigma(\mathcal{K}_\varphi)$. Therefore, $\sigma(\mathcal{K}_\varphi) = \sigma(K_\varphi) \cup \mathcal{R}(q_\varphi)$. The theorem is proved. □

3. Spectral analysis of the operators $\mathcal{K}_\varphi$ in dimension 1

This section is devoted to the 1D case, where the most advanced results have been obtained [10]. These results are also important for higher dimensional cases discussed below in Sect. 4. The reason is that the spectral estimations in higher dimensions have been obtained [13] through the reduction of the M-dimensional problem (under the specific extra conditions for the domain $\Omega \subset \mathbb{R}^M$ and the functional parameter $\varphi(\mathbf{x})$) to a countable set of 1D problems.

For the readers' convenience, this section is structured into several subsections. In Sect. 3.1 we discuss the Fourier transform, the adjoint operator, and the selfadjointness in the weighted space. Next, we turn to the study of the operators $\mathcal{K}_\varphi$ with acceptable equilibrium distribution functions $\varphi(x)$ having compact support $\Omega = (a, b)$. In Sect. 3.2 we introduce the appropriate reference operator $\mathcal{K}_0$ and develop its complete spectral analysis. In Sect. 3.3 we provide the results for $\mathcal{K}_\varphi$ corresponding to an acceptable equilibrium distribution function $\varphi(x)$ having the admissible support $\operatorname{supp}\varphi = \Omega$, using the resolvent comparison approach. Spectral estimations for the eigenvalues of $\mathcal{K}_\varphi$ are presented. We also discuss there the contribution of the complement to the support $\mathbb{R}\backslash\Omega$ to the spectrum of $\mathcal{K}_\varphi$ in the specific examples. In Subsection 3.4 we discuss one of the most physically interesting cases of the Gaussian equilibrium distribution function $\varphi(x)$ (which support is not compact, so it is not an acceptable function in the sense of Definition 1) and demonstrate that the spectral properties of the corresponding collision operator $\mathcal{K}_\varphi$ differ drastically from the case of the acceptable equilibrium distribution functions. Section 3.5 is devoted to the discussion on other spectral estimations for the operator $\mathcal{K}_\varphi$, obtained through the quadratic form approach. We also demonstrate there the non-negativity of the operators $\mathcal{K}_\varphi$ for a broad class of the equilibrium distribution functions $\varphi(x)$, establish links between the modified integral-difference operators and the weighted mean-square deviation functionals, and demonstrate a new property of the Legendre polynomials.

3.1. Dimension 1: Fourier transform, the adjoint operator, and the selfadjointness in the weighted space

Let us note [6, 10] that in the 1D case one cannot represent $\mathcal{K}_\varphi$ as a difference of two operators corresponding to two terms in the nominator, as the two corresponding integrals do not converge. Another important point is that $\mathcal{K}_\varphi$ is not an integral operator, as it is impossible to construct the corresponding integral kernel. However, it happens that under some simple conditions on $\varphi(x)$, the Fourier transform of $\mathcal{K}_\varphi$ is an integral operator [6, 10]. We use the Fourier representation in order to prove some important properties of the operators $\mathcal{K}_\varphi$. The following lemma is valid (see [10], Lemma 2.1).

Lemma 2. *For any real-valued function $\varphi(x) \in L_1(\mathbb{R}) \bigcap L_2(\mathbb{R})$, the operator $\mathcal{K}_\varphi$ acting in the space $L_2(\mathbb{R})$ obeys the relation*

$$\mathcal{K}_\varphi \circ \varphi = \varphi \circ \mathcal{K}_\varphi^* , \tag{15}$$

where $\mathcal{K}_\varphi^*$ is the adjoint operator with respect to the standard inner product in $L_2(\mathbb{R})$ and φ stands for the operator of multiplication by the function $\varphi(x)$.

Proof. is obtained [10] through the Fourier transform

$$\widehat{\mathcal{K}}_\varphi := F\, \mathcal{K}_\varphi\, F^{-1} ,$$
$$F(u) := \widehat{u}(k) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-ikx}\, u(x)\, dx .$$

One can calculate [6, 10] that $\widehat{\mathcal{K}}_\varphi$ is the integral operator with the weakly singular kernel

$$\widehat{\mathcal{K}}_\varphi(k,k') = \sqrt{\frac{2}{\pi}}\, \widehat{\varphi}(k-k') \left| \ln \left| \frac{k}{k-k'} \right| \right| ,$$

where $\widehat{\varphi}(k) := F(\varphi)$. The kernel of the adjoint operator $\mathcal{K}_\varphi^*$ can be obtained from the latter expression by the interchange of the arguments k, k' and the complex conjugation. As $\varphi(x) \in \mathbb{R}$, this results is

$$\widehat{\mathcal{K}}_\varphi^*(k,k') = \sqrt{\frac{2}{\pi}}\, \widehat{\varphi}(k-k') \left| \ln \left| \frac{k-k'}{k} \right| \right| .$$

The kernel of the operator $F(\mathcal{K}_\varphi \circ \varphi)$ is given by the convolution and can be calculated as

$$F(\mathcal{K}_\varphi \circ \varphi)(k,k') = \int_{-\infty}^{\infty} \widehat{\mathcal{K}}_\varphi^*(k,p)\, \widehat{\varphi}(p-k')\, dp = F(\varphi \circ \mathcal{K}_\varphi^*)(k,k').$$

Consequently, $\mathcal{K}_\varphi \circ \varphi = \varphi \circ \mathcal{K}_\varphi^*$. The lemma is proved. □

From Lemma 2 we obviously have the following corollary.

Corollary 1. *For any real-valued function $\varphi(x) \in L_2(\mathbb{R}) \cap L_2(\mathbb{R})$, the operator $\mathcal{K}_\varphi$ is selfadjoint in the weighted space $L_2(\mathbb{R}, dx/\varphi(x))$.*

Corollary 1 and its generalization to higher dimensions will be used to apply the quadratic forms approach (see Sect. 4 below).

3.2. Dimension 1: Reference operator

Now let us turn to the spectral analysis of the operators $\mathcal{K}_\varphi$, starting with the introduction and study of the reference operator. The reference operator $\mathcal{K}_0$ is a prototype for operators $\mathcal{K}_\varphi$ corresponding to the function $\varphi(x)$ with compact support $\Omega = (a,b) \subset \mathbb{R}$. Without loss of generality one can take $a = -1$, $b = 1$ using a simple linear change of variables $x \to x' = (2x - b - a)/(b - a)$ to get the equivalent problem on the renormalized real line such that $(a,b) \to (-1,1)$.

The operator $\mathcal{K}_0$ corresponds to the piecewise constant function

$$\chi_{[-1,1]}(x) := \begin{cases} 1\,, & x \in (-1,1)\,, \\ 0\,, & \text{otherwise}\,. \end{cases} \tag{16}$$

Obviously, $\chi_{[-1,1]}(x)$ is an acceptable function in the sense of Definition 1 and $(-1,1)$ is an admissible domain in the sense of Definition 2.

Let us note, that for 1D gas models the function $\varphi(x)$ plays the role of the equilibrium distribution (the probability density), so its natural normalization is $||\varphi||_{L_1(\Omega)} = 1$. It means that we should take $\varphi(x) = \chi_{[-1,1]}(x)/2$; however, it is more convenient to omit the factor 1/2 and use the formula (16) for $\varphi(x)$, which does not affect any further proofs.

Applying Lemma 1 to the case under consideration and performing simple calculations we get

$$\mathcal{K}_0^{\rm ii} := K_0 : u(x) \;\mapsto\; \int_{-1}^{1} \frac{u(x)\chi_{[-1,1]}(s) - u(s)\chi_{[-1,1]}(x)}{|x-s|}\, d, \quad x \in [-1,1]\,; \tag{17}$$

$$\mathcal{K}_0^{\rm ie} : u(s) \;\mapsto\; \int_{\mathbf{R}\setminus[-1,1]} \frac{u(s)}{|x-s|}\, ds, \quad x \in [-1,1]\,; \tag{18}$$

$$\mathcal{K}_0^{\rm ei} \equiv 0\,; \tag{19}$$

$$\mathcal{K}_0^{\rm ee} : u(\mathbf{x}) \;\mapsto\; q_0(x)\, u(x), \quad q_0(x) := \Big|\ln\Big|\frac{x-1}{x+1}\Big|\Big|\,. \tag{20}$$

To apply Theorem 1, we start with the study of the restricted operator K_0 given by formula (17). We recall the following result first obtained in [6] (see also [10], Theorem 3.2).

Theorem 2. *The operator K_0 in the Hilbert space $L_2[-1,1]$ is selfadjoint, $K_0^* = K_0$, and its spectrum $\sigma(K_0)$ is discrete and equals to the set of simple eigenvalues μ_n,*

$$\sigma(K_0) = \{\mu_n\}_{n=0}^{\infty}\,, \tag{21}$$

where

$$\mu_0 = 0\,, \quad \mu_n = 2\sum_{n=1}^{j} \frac{1}{j}\,, \quad n \geq 1\,. \tag{22}$$

The corresponding eigenfunctions are the (normalized) Legendre polynomials:

$$p_0(x) = \frac{1}{2}\,, \quad p_n(x) = \sqrt{\frac{2n+1}{2}}\,\frac{1}{2^n n!}\,\frac{d^n}{dx^n}(x^2+1)^n\,, \quad n \geq 1\,. \tag{23}$$

Proof. The proof is given in [6, 10]. Here we just outline its key points. The selfadjointness of the operator K_0 follows from Lemma 2. Indeed, in our case $\varphi(x) = \chi_{[-1,1]}(x)$, and due to Lemma 2 we have $\mathcal{K}_0 \circ \chi_{[-1,1]} = \chi_{[-1,1]} \circ \mathcal{K}_0^*$. The operator of the multiplication by the indicator $\chi_{[-1,1]}(x)$ is the projection operator $\mathcal{P}_{\rm i}$, therefore $\mathcal{K}_0\mathcal{P}_{\rm i} = \mathcal{P}_{\rm i}\mathcal{K}_0^*$, which implies

$$K_0 = \mathcal{P}_{\rm i}\mathcal{K}_0\mathcal{P}_{\rm i} = \mathcal{P}_{\rm i}\mathcal{K}_0^*\mathcal{P}_{\rm i} = K_0^*\,. \tag{24}$$

Next, polynomials of the order n, $\widetilde{p}_n(x) = \sum_{j=0}^{n} b_j^{(n)} x^n$ are considered and it is shown [6, 10] that one can uniquely choose the coefficients $b_j^{(n)}$ such that $b_n^{(n)} \neq 0$ and $K_0\widetilde{p}_n = \mu_n\widetilde{p}_n$. Therefore, the set $\{\mu_n\}_{n=0}^{\infty}$ is in the discrete spectrum of the operator K_0 and the corresponding eigenfunctions are the polynomials $\widetilde{p}_n(x)$. As $K_0 = K_0^*$, the polynomials $\widetilde{p}_n(x)$ are the Legendre polynomials $\widetilde{p}_n(x) \equiv p_n(x)$, which completes the proof. □

Now we are ready to describe the spectrum of the reference operator $\mathcal{K}_0$ [6, 10] applying Theorem 1. The discrete spectrum generated by the restricted operator K_0 is given by Theorem 2. Image $\mathcal{R}(q_0)$ of the function $q_0(x)$ given by formula (20) fills the positive semiaxis $\mathbb{R}_+$ with double multiplicity, i.e. for any $\lambda > 0$ there are two inverse images $x_\lambda^\pm$: $q_0(x_\lambda^\pm) = \lambda$, where

$$x_\lambda^\pm = \mp \frac{1+e^\lambda}{1-e^\lambda}\,, \tag{25}$$

so $x_\lambda^+ > 1$ and $x_\lambda^- < -1$.

Therefore, with Theorem 1 we get the following statement, first obtained in [6] (see also [10, Theorem 3.3]).

Theorem 3. *The spectrum $\sigma(\mathcal{K}_0)$ of the operator $\mathcal{K}_0$ in the Hilbert space $L_2(\mathbb{R})$ fills the positive semiaxis $\mathbb{R}_+$. It is the union of the discrete spectrum $\sigma_d(\mathcal{K}_0) = \sigma(K_0) = \{\mu_n\}_{n=0}^{\infty}$, where μ_n are the (simple) eigenvalues given by formula* (22), *and the absolute-continuous spectrum of double multiplicity $\sigma_{ac}(\mathcal{K}_0) = \mathbb{R}\backslash\sigma(\mathcal{K}_0)$. The eigenfunctions corresponding to the eigenvalues μ_n are*

$$u_n(x) = \chi_{[-1,1]}(x)\, p_n(x)\,. \tag{26}$$

The generalized eigenfunctions corresponding to points $\lambda \in \sigma_{ac}(\mathcal{K}_0) = \mathbb{R}_+\backslash\sigma(\mathcal{K}_0)$ are

$$u_\lambda^\pm(x) = \chi_{[-1,1]}(x)\, u_0^{\lambda\pm}(x) + \delta(x - x_\lambda^\pm)\,, \tag{27}$$

where

$$u_0^{\lambda\pm}(x) := (K_0 - \lambda)^{-1}\big(|x - x_\lambda^\pm|^{-1}\big) = -\sum_{n\geq 0} p_n(x_\lambda^\pm)\, p_n(x) \in L_2[-1,1]\,. \tag{28}$$

Proof. It can be find in [6, 10]. Here we just note that the last equality in formula (28) coming by the straightforward calculation follows from the fact that Legendre polynomials $p_n(x)$ are the eigenfunctions of the restricted operator $K_0 = K_0^*$ (see Theorem 3), thus the resolvent of the operator K_0 can be presented as

$$(K_0 - z)^{-1} = \sum_{n\geq 0} \frac{p_n\langle\cdot, p_n\rangle_{L_2[-1,1]}}{\mu_n - z}\,. \tag{29}$$

We have shown that both the spectrum $\sigma(K_0)$ of the restricted operator K_0 and its complement $\mathbb{R}_+\backslash\sigma(\mathcal{K}_0)$ are the subsets of the spectrum $\sigma(\mathcal{K}_0)$ of the reference operator $\mathcal{K}_0$, which means that $\mathbb{R}_+ \subset \sigma(\mathcal{K}_0)$. On the other hand, the spectrum of the operator K_0 is nonnegative. Therefore, if $\lambda \notin \mathbb{R}_+$ and $\lambda \in \sigma(\mathcal{K}_0)$, the equation $q_0(x)u_\lambda(x) = \lambda u_\lambda(x)$ should be satisfied with some nontrivial function

$u_\lambda(x)$. However, that is impossible, because the image of the function $q_0(x)$ is positive, $\mathbb{R}(q_0) \subset \mathbb{R}_+$. Therefore, $\sigma(\mathcal{K}_0) \subset \mathbb{R}_+$ and finally we have $\sigma(\mathcal{K}_0) = \mathbb{R}_+$. The theorem is proved. □

Remark 3. (Link to the differential operator generating the Legendre polynomials)

As mentioned in [7, 10], Theorem 3 implies that the operator K_0 commutes with the operator $\mathcal{L} = (x^2-1)(d^2/dx^2) + 2x(d/dx)$ generating the Legendre polynomials, $\mathcal{L} \circ K_0 - K_0 \circ \mathcal{L} = 0$. This can be also checked by a straightforward independent calculation for every monomial x^n. The eigenvalues of the operator L are $n(n+1)$. Using the representation [34] for $\sum_{j=1}^n 1/j$, one can get the following relation between the operators K_0 and $\mathcal{L}$:

$$K_0 = 2CI + 2\ln G + G^{-1} = 2\sum_{k=2}^{\infty} A_k G^{-1}(G+I)^{-1}\cdots(G+(k-1)I)^{-1}$$

where $G := (1/2)(I+4\mathcal{L})^{1/2} - I$, $A_k := k^{-1}\int_0^1 x(1-x)(2-x)\cdots(k-1-x)dx$.

3.3. Dimension 1: Spectral structure and spectral estimations for the operator $\mathcal{K}_\varphi$ corresponding to an acceptable equilibrium distribution function $\varphi(x)$

Basing on the results described above (see Sects. 3.1 and 3.2) one can turn to the spectral analysis of the operators $\mathcal{K}_\varphi$ in the 1D case. The following result was first obtained in [6] (see also [10, Theorem 3.4]).

Theorem 4. *If the function $\varphi(x)$ is an acceptable function in the sense of Definition 1 and its support is $\Omega = (a,b) \subset \mathbb{R}$, then the spectrum $\sigma(\mathcal{K}_\varphi)$ of the corresponding operator $\mathcal{K}_\varphi$ in the Hilbert space $L_2(\mathbb{R}, dx/\varphi(x))$ fills the positive semiaxis $\mathbb{R}_+$ being the union*

$$\sigma(\mathcal{K}_\varphi) = \sigma_{ac}(\mathcal{K}_\varphi) \cup \sigma_d(\mathcal{K}_\varphi)\,, \tag{30}$$

where the discrete spectrum $\sigma_d(\mathcal{K}_\varphi) = \sigma(K_\varphi) = \{\tau_n\}_{n=0}^\infty$ ($\tau_n \to \infty$ when $n \to \infty$) coincides with the spectrum of the restricted operator $K_\varphi = \mathcal{P}_{\rm ii}\mathcal{K}_\varphi\mathcal{P}_{\rm ii}$. Here $\mathcal{P}_{\rm ii}$ is the projection on the subspace $L_2([a,b];\, dx/\varphi(x))$. If $\lambda \in \mathbb{R}_+ \backslash \sigma(K_\varphi)$, then $\lambda \in \sigma_{ac}(\mathcal{K}_\varphi)$ is a point of absolutely-continuous spectrum having double multiplicity and the corresponding generalized eigenfunctions are

$$u^\pm_{\varphi,\lambda}(x) = \chi_{[a,b]}(x)\,(K_\varphi - \lambda)^{-1}\left(\frac{\varphi(x)}{|x - x^\pm_{\varphi,\lambda}|}\right) + \delta(x - x^\pm_{\varphi,\lambda})\,, \tag{31}$$

where $x^\pm_{\varphi,\lambda}$ are the two inverse images of the function $q_\varphi(x) = \displaystyle\int_a^b \varphi(s)|x-s|^{-1}\,ds$ in the point λ: $q_\varphi(x^\pm_{\varphi,\lambda}) = \lambda$, $x^-_{\varphi,\lambda} < a$, $x^+_{\varphi,\lambda} > b$.

Proof. The proof was first obtained in [6] (see also [10, Theorem 3.4]). Regarding the absolute-continuous spectrum $\sigma_{ac}(\mathcal{K}_\varphi) = \mathcal{R}\big(q_\varphi(x)\big)$, it essentially repeats the proof of Theorem 3 for the reference operator $\mathcal{K}_0$. In particular, the operator

K_φ is selfadjoint in the space $L_2([a,b];\, dx/\varphi(x))$. Consequently, its spectrum is real. Note, that the spaces $L_2([a,b];\, dx/\varphi(x))$ and $L_2[a,b]$ are isomorphic (see Remark 4 below). As mentioned above, by linear change of variables, without losing generality, we can assume that $a=-1, b=1$. Hereafter in this proof, we accept this assumption.

To deal with the discrete spectrum $\sigma_d(\mathcal{K}_\varphi) = \sigma(K_\varphi)$, by straightforward calculation one can get

$$K_\varphi = \varphi \circ K_0 - (K_0\varphi)\,, \tag{32}$$

where φ and $(K_0\varphi)$ stand for the operators of the multiplication by the functions $\varphi(x)$ and $(K_0\varphi)(x)$ respectively.

We denote by $R_0(z) := (K_0 - z)^{-1}$ and $R_\varphi(z) := (K_\varphi - z)^{-1}$ the resolvents of the operators K_0 and K_φ respectively. One can check that the following relation is valid:

$$R_\varphi(z) = R_0(z)\circ\frac{1}{\varphi} - R_\varphi(z)\circ\big[z(\varphi - I)\,\varphi - (K_0\varphi)\big]\circ R_0(z)\circ\frac{1}{\varphi}\,. \tag{33}$$

Therefore,

$$R_\varphi(z) = R_0(z)\circ\frac{1}{\varphi}\circ\left[I + \big[z(\varphi - I)\,\varphi - (K_0\varphi)\big]\circ R_0(z)\circ\frac{1}{\varphi}\right]^{-1} \tag{34}$$

if the inverse operator in the right-hand side of the formula (34) exists. The resolvent $R_0(z)$ of the reference operator has a discrete spectrum with the eigenvalues $(\mu_n - z)^{-1}$ and is a compact operator except for the countable discrete set $\{z = \mu_n\}_{n\geq 0}$. Due to the conditions (5) and (6), the operators of the multiplication by the functions $\varphi(x)$, $1/\varphi(x)$ and $(K_0\varphi)(x)$ are bounded. Therefore, the operator $\big[z(\varphi - I)\,\varphi - (K_0\varphi)\big]\circ R_0(z)\circ\frac{1}{\varphi}$ is compact except for the countable discrete set $\{z = \mu_n\}_{n\geq 0}$, because it is the product of a compact operator and bounded operators [1, 2] outside of this set. Hence, its spectrum cannot have an accumulation point at $\lambda = -1$. Outside of the mentioned set, it is an analytic operator-valued function of z. Consequently, the point $\lambda = -1$ can be an eigenvalue of this operator only for a countable discrete set of z. Therefore, outside of this set, there exists a bounded operator $\left[I + \big[z(\varphi - I)\,\varphi - (K_0\varphi)\big]\circ R_0(z)\circ\frac{1}{\varphi}\right]^{-1}$. Then in the right-hand side of the formula (34), we have the product of this bounded operator and the compact operator $R_0(z)\circ\frac{1}{\varphi}$. Hence, the resolvent $R_\varphi(z)$ is a compact operator except for a countable discrete set of z. This implies that the operator K_φ can have only a discrete spectrum and its eigenvalues $\tau_n \to \infty$ when $n \to \infty$. These eigenvalues form the discrete spectrum $\sigma_d(\mathcal{K}_\varphi)$ of the operator $\mathcal{K}_\varphi$. The theorem is proved. □

Now, following [6, 10], under the conditions of Theorem 4 we can obtain the spectral estimations for the operator $\mathcal{K}_\varphi$. For the domain $\Omega := \operatorname{supp}\varphi = (a,b)$ the restricted operator $K_\varphi = \mathcal{P}_{\mathrm{ii}}\mathcal{K}_\varphi\mathcal{P}_{\mathrm{ii}}$ generates the discrete spectrum $\sigma_d(\mathcal{K}_\varphi) =$

$\sigma(K_\varphi) = \{\tau_n\}_{n=0}^{\infty}$ of the operator $\mathcal{K}_\varphi$. Again, without using generality, we can assume that $a = -1$, $b = 1$.

Corollary 1 and Theorem 4 imply that the operators K_0 and K_φ are self-adjoint in the Hilbert spaces $L_2[-1,1]$ and $L_2([-1,1], dx/\varphi(x))$, respectively. We denote the inner products and the norms in these spaces respectively as

$$(u,v) := \int_{-1}^{1} u(x)\bar{v}(x)\,dx\,; \qquad ||u|| := \sqrt{(u,u)}\,; \tag{35}$$

$$\langle u,v\rangle_\varphi := \int_{-1}^{1} u(x)\bar{v}(x)\,\frac{dx}{\varphi(x)}\,; \qquad \mathbf{I}u\mathbf{I}_\varphi := \sqrt{\langle u,u\rangle_\varphi}\,. \tag{36}$$

Let us make the following important remark.

Remark 4. (Isomorphism of spaces $L_2[a,b]$ and $L_2([a,b];\, dx/\varphi(x)))$

For any acceptable function $\varphi(x)$ having an admissible (compact) support $\Omega = (a,b)$ the restricted Hilbert spaces $L_2[a,b]$ and $L_2([a,b];\, dx/\varphi(x)$ are isomorphic. Indeed, due to the conditions (5) and (6), for the norms $||u||$ in $L_2[a,b]$ and $\mathbf{I}u\mathbf{I}_\varphi$ in $L_2([a,b];\, dx/\varphi(x)$ we have

$$\Big(\varepsilon_\varphi + (b-a)\,A_\varphi\Big)\,||u|| \le \mathbf{I}u\mathbf{I}_\varphi \le \varepsilon_\varphi^{-1}\,||u||\,.$$

We consider the spectral problem

$$u_n(x) = p_n(x) - 2\delta \sum_{m\neq n} \frac{((K_0-\mu_n)\,h, p_n p_m)}{\mu_n - \mu_m}\, p_m(x) + o(\delta)\,. \tag{37}$$

Now let us consider the continuous spectrum of the operator $\mathcal{K}_\varphi$, generated by the complement to the support of the equilibrium distribution function $\varphi(x)$. As one can see from the previous discussion, the support of the equilibrium distribution function $\operatorname{supp}\varphi$ is "responsible" for the discrete spectrum of the operator $\mathcal{K}_\varphi$ (coinciding with the spectrum of the restricted operator K_φ), while the complement to the support $\mathbb{R}\backslash\operatorname{supp}\varphi$ "generates" the branches of the continuous spectrum given by the image of the function $q_\varphi(x)$ when $x \notin \operatorname{supp}\varphi$. As shown in [10] (see Sect. 3.6 there), every interval, where the equilibrium distribution function $\varphi(x)$ vanishes, generates a branch of continuous spectrum of the corresponding operator $\mathcal{K}_\varphi$. As shown above (see Theorem 4), the image $\mathcal{R}(q_\varphi)$ of the function $q_\varphi(x)$, $x \notin \operatorname{supp}\varphi$, generates the absolutely continuous spectrum $\sigma_{ac}(\mathcal{K}_\varphi)$ of the operator $\mathcal{K}_\varphi$. Different cases were illustrated in [10] with several specific examples. Briefly, the results are as follows.

Example 1. (Absolutely continuous spectrum of infinite multiplicity)

Let the equilibrium distribution function $\varphi(x)$ be

$$\varphi(x) = \begin{cases} 2^{-n-2}\,, & x \in [2n, 2n+1]\,,\ n \ge 1; \\ 2^{2n-2}\,, & x \in [2n-1, 2n]\,,\ n \le -1; \\ 2^{-2}\,, & x \in [-1,1]\,; \\ 0\,, & \text{otherwise}\,. \end{cases} \tag{38}$$

One can easily calculate $\int_{-\infty}^{\infty} \varphi(x)\,dx = \sum_{n\geq 0} 2^{-n} = 1$. Note, that in this case the function $\varphi(x)$ does not have a compact support. As shown in [10], the corresponding function

$$q_\varphi(x) := \int_{\mathbf{R}\backslash \mathrm{supp}\,(\varphi)} \varphi(s)\,|x-s|^{-1}\,ds\,, \quad x \in \mathbb{R}\backslash \mathrm{supp}\,\varphi$$

maps the interval $[2j-1, 2j]$ into the semi-infinite interval $[M_j, \infty)$, where $0 < M_j = O\big(|j|^{-1}\big)$ at $j \to \infty$. The same is true for $j < 0$. It means that the open semiaxis $(0, \infty)$ belongs to the absolute continuous spectrum of the operator $\mathcal{K}_\varphi$ and has the infinite spectral multiplicity.

Example 2. (A branch of the absolutely continuous spectrum parametrically shrinking)

Here we consider the equilibrium distribution function defined as

$$\varphi(x) = \begin{cases} \left[\ln \frac{a+1}{a-1}\right]^{-1} \frac{1}{x+a}\,, & x \in [-1,1]\,; \\ 0\,, & \text{otherwise}\,. \end{cases} \tag{39}$$

If $a > 1$, then $0 < \varphi(x) \in L_1(\mathbb{R})$ and $||\varphi(x)||_{L_1} = 1$. One can calculate [10]

$$q_\varphi(x) = \int_{-1}^{1} \varphi(x)\,|x-s|\,ds = -\frac{1}{x+a} \tag{40}$$

and see that in the image of the function $q_\varphi(x)$ is

$$\mathcal{R}(q_\varphi) = \Big(-\frac{1}{a+1}, \frac{1}{a-1}\Big)\,.$$

Therefore, at $a \to 1+0$ and $a \to +\infty$ we have $\mathcal{R}(q_\varphi) \to (-1/2, +\infty)$ and $\mathcal{R}(q_\varphi) \to (-1/a, 1/a)$, respectively, i.e., the branch of the continuous spectrum shrinks as $a \to +\infty$.

Example 3. (A finite branch of the absolutely continuous spectrum)

Here we consider the case of continuous equilibrium distribution function

$$\varphi(x) = \begin{cases} x+1\,, & x \in [-1,0]\,; \\ -x+1\,, & x \in [0,1]\,; \\ 0\,, & \text{otherwise}\,. \end{cases} \tag{41}$$

One can calculate [10]

$$q_\varphi(x) = |x|\,\ln(1-1/x^2) + \Big|\ln\Big|\frac{x+1}{x-1}\Big|\Big|\,. \tag{42}$$

Therefore, the image of the function $q_\varphi(x)$ is the interval $[0, 2\ln 2]$ and has in this interval double multiplicity.

Remark 5. (Link to Jacobi matrices)

As mentioned in [10], for the specific choice of the functions $\varphi(x)$ a link of the spectral problem under investigation with Jacobi matrices having unbounded entries [25, 26] can be traced. Namely, let us take as $\varphi(x)$ the normalized Legendre polynomial $\varphi(x) \equiv p_k(x)$. Of course, it is not an acceptable function in the sense of Definition 1, but that is not significant for tracing the mentioned link.

Decomposition of the function $u(x)$ in the normalized Legendre polynomials $p_k(x)$, $u(x) = \sum_{k=0}^{\infty} u_k\, P_k(x)$, for $\varphi(x) \equiv p_k(x)$ turns the spectral problem $K_\varphi u = \tau u$ in the Hilbert space $L_2[-1,1]$ into the following spectral problem in the Hilbert space l_2^+:

$$J^{(l)}\,\hat{u} = \tau\,\hat{u}\,, \tag{43}$$

where $\hat{u} := (u_0, u_1, \dots)^T$ and the entries of the matrix $J^{(l)}$ are

$$J^{(l)}_{km} = (\mu_k - \mu_l)\,\gamma_{klm}\,, \tag{44}$$

where

$$\gamma_{klm} := \int_{-1}^{1} p_k(x)\,p_l(x)\,p_m(x)\,dx\,.$$

Obviously $\gamma_{klm} \neq 0$ only if $k+m \leq l$, $k+l \leq m$, $l+m \leq k$ simultaneously, which means that $-l \leq m-k \leq l$ and $m+k \geq l$. Hence, $J^{(l)}$ is a $(2l+1)$-diagonal semi-infinite matrix. In the simplest case, $l=1$, $J^{(1)}$ is the 3-diagonal Jacobi matrix having the entries

$$J^{(1)}_{km} = (\mu_k - 2)\int_{-1}^{1} p_k(x)\,p_m(x)\,x\,dx\,.$$

3.4. Dimension 1: the Gaussian equilibrium distributions

Contrary to most of the above-considered cases, physically important Gaussian equilibrium distributions [3, 8, 9, 10] have infinite support. They are not acceptable functions in the sense of Definition 1 due to the violation of the condition (6) and the corresponding operators $\mathcal{K}_\varphi$ cannot be analyzed using the above described technique. The main technical reason is that in this case the operator of the multiplication by the function $1/\varphi(x)$ is not bounded, so the resolvent comparison approach used in Theorem 4 (see Sect. 3.3 above) fails.

It was shown that the violation of the condition (6) drastically changes the spectral structure of the operator $\mathcal{K}_\varphi$. First numerical [8] and later analytical [9, 10] studies have shown it for the Gaussian equilibrium distribution functions. Namely, there was considered the family of the operators corresponding to the truncated to the interval $[-a,a]$ Gaussian equilibrium distribution function $\varphi_{a,\beta}(x) := \Gamma_{a,\beta}\,\chi_{[-a,a]}(x)\,e^{-\beta^2 x^2}$, where $\Gamma_{a,\beta}$ is the normalizing coefficient,

$$\Gamma^{-1}_{a,\beta} := \int_{-a}^{a} e^{-\beta^2 x^2}\,dx = \sqrt{\pi}\beta^{-1}\mathrm{erf}(\beta a).$$

Without loss of generality, one can take $\beta = 1$, thus coming to the operators $\mathcal{K}_G^{[a]} := \mathcal{K}_{\varphi_a}$ corresponding to the truncated Gaussian equilibrium distribution functions

$$\varphi_a(x) := \begin{cases} \Gamma_a\,e^{-x^2}\,,\ \Gamma_a^{-1} := \sqrt{\pi}\,\mathrm{erf}(a)\,, & x \in (-a,a)\,; \\ 0\,, & \text{otherwise}\,. \end{cases} \tag{45}$$

Infinite integration limits in the original operator (1), $M = 1$, are always understood as the limit of the integral over the interval $[-a, a]$ when $a \to \infty$. One can have an intuitive feeling [3] that, as truncated Gaussian functions are "very similar" for different but large values of the truncation parameter a, and the spectral properties of the corresponding operators $\mathcal{K}_G^{[a]}$ will also be similar for different large values of a. However, that is not true [9, 10]. Namely, there is no regular limit of the operator $\mathcal{K}_G^{[a]}$ at $a \to \infty$. Therefore, there is no way to develop a successful perturbation theory for the spectrum of the operator $\mathcal{K}_G^{[a]}$ with respect to the parameter $1/a$, and the spectral properties of the corresponding operator change drastically when $a = \infty$. That is related to the obvious fact that the spectral problem $\mathcal{K}_G^{[a]} u = \lambda u$ is equivalent to the spectral problem $\widetilde{\mathcal{K}}_G^{[a]} u = \lambda u$, where the operator $\widetilde{\mathcal{K}}_G^{[a]} \mathcal{P}_{[-1,1]}$ corresponds to the equilibrium distribution function

$$\widetilde{\varphi}_a(x) := \begin{cases} \Gamma_a \, e^{-a^2 x^2} , & x \in [-1, 1] ; \\ 0 , & \text{otherwise} , \end{cases} \tag{46}$$

got by the change of variables $x \to x/a$.

Next we consider the restricted operators $\widetilde{K}_G^{[a]} = \mathcal{P}_{[-1,1]} \widetilde{\mathcal{K}}_G^{[a]} \mathcal{P}_{[-1,1]} \mathcal{P}_{[-1,1]}$ and $K_G^{[a]} = \mathcal{P}_{[-a,a]} \mathcal{K}_G^{[a]} \mathcal{P}_{[-a,a]}$ generating the discrete spectra of the operators $\widetilde{\mathcal{K}}_G^{[a]}$ and $\mathcal{K}_G^{[a]}$, respectively. In the limit case $a = \infty$ we observe for the operator $K_G^{[\infty]} = \mathcal{P}_{[-a,a]} \, \widetilde{\mathcal{K}}_G^{[\infty]} \, \mathcal{P}_{[-a,a]}$ (and, consequently, for $K_G^{[\infty]}$) the spectral concentration in the vicinity of zero. More specifically, let us denote by $E_a[-S, S]$ the spectral operator-valued measure [1, 2] of the operator $\widetilde{\mathcal{K}}_G^{[a]}$ on the interval $[-S, S]$. By $\mathcal{H}_a$ we denote the Hilbert space $\mathcal{H}_a := L_2([-1, 1], dx/\widetilde{\varphi}_a(x))$ where the operator $\widetilde{\mathcal{K}}_G^{[a]}$ acts as a selfadjoint operator. The main relevant result [9, 10] is the following theorem.

Theorem 5. *For any $S > 0$,*

$$\dim(E_a[-S, S] \, \mathcal{H}_a) \to \infty \quad \textit{when } a \to \infty . \tag{47}$$

This theorem means that the number of the eigenvalues (counted with their multiplicity) of the operator $\widetilde{\mathcal{K}}_G^{[a]}$ (and, consequently, of the operator $K_G^{[a]}$) in an arbitrary small vicinity of zero increases to infinity when the truncation parameter a goes to infinity. Indeed, due to Theorem 4, the spectra of these operators are purely discrete for all $a < \infty$. Hence, the increase of the spectral measure on the interval $[-S, S]$ can be caused only by the increase of the number of the eigenvalues (counted with their multiplicity) on this interval. Therefore, $\lambda = 0$ is the point of the spectral concentration for the limit operator $K_G^{[\infty]}$.

Proof. of this theorem is heavy and rather technical [9, 10] (see [10, Theorem 4.1]). Here we just outline the key points of this proof. In order to prove the theorem using the bilinear form approach it is enough [1, 2] to construct for all integers $N > 0$ a linear set $F_N^a \subset \mathcal{D}_{\widetilde{\varphi}_a}$, $\dim(F_N^a) = N$ such that for any $S > 0$ there exists the parameter $a_0(N,S)$ such that for all $a > a_0(N,S)$ the inequality

$$\left|\langle\widetilde{\mathcal{K}}_G^{[a]}u,u\rangle\right| \le S\,|\langle u,u\rangle_{\widetilde{\varphi}_a}| \tag{48}$$

is true for all $u \in F_N^a$. We construct F_N^a as the linear span

$$F_N^a = \bigvee_{k=0}^{N-1} u_k^{[a]}\,,\ u_k^{[a]}(x) := p_k(x)\,\widetilde{\varphi}_a^{1/2}(x)\,, \tag{49}$$

where $p_k(x)$ are the Legendre polynomials normalized in the space $L_2[-1,1]$ (the eigenfunctions of the reference operator K_0). The functions $u_k^{[a]}(x)$ are orthogonal in the Hilbert space $L_2([-1,1], dx/\widetilde{\varphi}_a(x))$. Therefore, $\dim F_N^a = N$ for all a and any function $u \in F_N^a$ can be represented as $u(x) = \sum_{k=0}^{N-1} \alpha_k\, u_k^{[a]}(x)$. Obviously,

$$\left|\langle u,u\rangle\right|_{\widetilde{\varphi}_a} = \sum_{k=0}^{N-1} |\alpha_k|^2\,. \tag{50}$$

We use the representation (32) for the operator $\widetilde{\mathcal{K}}_G^{[a]}$ and get

$$\left\langle\widetilde{\mathcal{K}}_G^{[a]}u,u\right\rangle_{\widetilde{\varphi}_a} = (K_0u,u) - \left\langle(K_0\widetilde{\varphi}_a(x))u,u\right\rangle_{\widetilde{\varphi}_a}\,. \tag{51}$$

We estimate the two terms in the right-hand side of Eq. (51) separately. Following [9, 10] (see [10, Theorem 4.1]), when estimating the term (K_0u,u) we split the domain of integration $\Omega = (-1,1) \ni s$ in two parts: $\Omega_1^{[a]}(x) := \left\{s \in \Omega :\ |x-s| < a^{-1/2}\right\}$ and $\Omega_2^{[a]}(x) := \left\{s \in \Omega :\ |x-s| \ge a^{-1/2}\right\}$. For the estimation both terms in the right-hand side of Eq. (51), we use the Laplace method [27] to calculate the asymptotics of the integrals and get the following result for the first term:

$$|(K_0u,u)| \le \mathcal{G}_1(N)a^{-1/2}\sum_{k=0}^{N-1}|\alpha_k|^2\left(1+O(a^{-1})\right), \tag{52}$$

where the coefficient

$$\mathcal{G}_1(N) = \frac{4N^2(1+\sqrt{2}e^{-1/2}}{\operatorname{erf}(1)}\max_{0\le k\le N-1}\max_{x\in[-1,1]}|p_k(x)|^2$$

does not depend on a and is finite for any $N < \infty$. For the second term in the right-hand side of Eq. (51) the result is:

$$\left|\langle(K_0\widetilde{\varphi}_a(x))u,u\rangle\right|_{\widetilde{\varphi}_a} \le \mathcal{G}_2(N)\,a^{-1}\sum_{k=0}^{N-1}|\alpha_k|^2\left(1+O(a^{-1})\right), \tag{53}$$

where the coefficient

$$\mathcal{G}_2(N) := \frac{4N^2}{\sqrt{\pi}\operatorname{erf}(1)}\sum_{m=0}^{2N-2}\mu_m|p_m(0)|\max_{0\le k\le N-1}\max_{0\le l\le N-1}|\gamma_{klm}|$$

does not depend on a and is finite for any $N < \infty$. Here

$$\gamma_{klm} := \int_{-1}^{1} p_k(x)p_l(x)p_m(x)\,dx\,.$$

Formulae (50)–(53) imply that that for any $N > 0$, any $S > 0$, and any function $u \in F_N^a$, the inequality (48) is true for sufficiently large $a > a_0(N,S)$. Taking into account the normalization of the Legendre polynomials $p_k(x)$ in the Hilbert space $L_2[-1,1]$, we get a very rough estimate

$$a_0(N,S) \le \Big(\frac{4(1+\sqrt{2}e^{-1/2})}{\operatorname{erf}(1)}\,\frac{N^3}{S}\Big)^2\,. \tag{54}$$

The theorem is proved. □

3.5. Dimension 1: Quadratic form approach, links to the mean-value functionals and a new property of the Legendre polynomials

In this subsection we discuss the recent results [13] based on the application of the quadratic form approach [1, 2] to the problems under consideration.

We focus in the discrete spectrum and thus consider the restricted operators K_φ. We introduce the modified operators

$$Q_\varphi := \frac{1}{2}\varphi(x) \circ K_\varphi\,. \tag{55}$$

Using the representation (32) the modified operators (55) can be represented as

$$Q_\varphi = \frac{1}{2}\,K_0 - V_\varphi\,, \tag{56}$$

where V_φ stands for the operator of multiplication by the function

$$V_\varphi(x) = \frac{(K_0\varphi)(x)}{2\varphi(x)}\,. \tag{57}$$

The function $V_\varphi(x)$ is called as the *effective potential*. We assume that $\varphi(x)$ is an acceptable function. To be specific, without losing generality, we also assume that $\Omega = \operatorname{supp}(\varphi) = (-1,1)$.

Let us introduce the quadratic form

$$\varkappa_\varphi[u] := \frac{1}{2}\,\langle K_\varphi u, u\rangle_\varphi = (Q_\varphi u, u)\,. \tag{58}$$

Study of this quadratic form allows for important conclusions on the properties of the modified operators Q_φ [13]. In particular, the following statement is true (see [13], Theorem 1):

Theorem 6. *For any acceptable equilibrium distribution function $\varphi(x)$, the quadratic form $\varkappa_\varphi[u]$ is nonnegative, $\varkappa_\varphi[u] \ge 0$, with the sharp lower boundary $m(\varkappa_\varphi) = 0$ achieved with $u(x) \equiv \varphi(x)$: $\varkappa_\varphi[\varphi] = 0$.*

Proof. The claim is proved in [13] using the representation (56). The terms (K_0u, u) and $(V_\varphi u, u)$ are estimated separately. For both terms, decomposing the domain of integration (square $\{x, s : -1 \le x, s \le 1\} \subset \mathbb{R}^2$) in two triangles: $\Delta_1 \subset \mathbb{R}^2$ where $-1 \le s \le x \le 1$ and $\Delta_2 \subset \mathbb{R}^2$ where $= 1 \le x < s \le 1$, and changing variables $x \leftrightarrow s$ in the integral over Δ_2, one gets [13]

$$\varkappa_\varphi[u] = \frac{1}{2} \iint_{\Delta_1} \frac{dx\,ds}{|x-s|} \frac{|u(x)\varphi(s) - u(s)\varphi(x)|^2}{\varphi(x)\,\varphi(s)} \ \ge\ 0\,. \tag{59}$$

Obviously, $\varkappa[\varphi] = 0$, which finishes the proof of the theorem. □

Theorem 6 together with minimal principle for quadratic forms [1, 2] of operators means the nonnegativity of the operators Q_φ, i.e., $\sigma(Q_\varphi) \subseteq \mathbb{R}_+$.

In [13] the following bilateral estimation for the quadratic form $\varkappa_\varphi[u]$ was obtained:

$$\frac{1}{2}\,(K_0u, u) - \frac{A_\varphi}{4\,\varepsilon_\varphi}\,||u||^2 \le \varkappa_\varphi[u] \le \frac{1}{2}\,(K_0u, u) + \frac{A_\varphi}{4\,\varepsilon_\varphi}\,||u||^2\,. \tag{60}$$

This implies the following bilateral estimations for the eigenvalues of the operator K_φ (see [13], Theorem 2):

Theorem 7. *For any acceptable function $\varphi(x)$, the eigenvalues ν_n^φ of the corresponding operator Q_φ lie in the intervals*

$$\frac{1}{2}\,\mu_n - \frac{A_\varphi}{4\,\varepsilon_\varphi} \le \nu_n^\varphi \le \frac{1}{2}\,\mu_n + \frac{A_\varphi}{4\,\varepsilon_\varphi}\,. \tag{61}$$

The expression (59) for the quadratic form $\varkappa_\varphi[u]$ can be rewritten [13] in terms of the function $w_\varphi(x) := u(x)/\varphi(x)$,

$$\widetilde{\varkappa}_\varphi[w] := \varkappa_\varphi[w\,\varphi] = \frac{1}{4} \int_{-1}^{1}\int_{-1}^{1} \frac{|w(x) - w(s)|^2}{|x-s|}\,dx\,ds\,. \tag{62}$$

Due to the minimal principle [1, 2], this implies the following theorem (see [13, Theorem 3]).

Theorem 8. *For any acceptable function $\varphi(x)$, the eigenfunctions $\widetilde{u}_n(x)$ and eigenvalues ν_n^φ of the operator Q_φ can be calculated through the minimization of the weighted mean-square functional defined by formula* (62)*, under the condition*

$$w_n(x) \perp \bigvee_{l=0}^{n-1} w_l\,, \quad w_0(x) \equiv 1\,, \tag{63}$$

where $\widetilde{u}(x) \equiv w(x)\,\varphi(x)$ and the orthogonality is with respect to the inner product

$$\langle w, v\rangle_{\varphi^{-2}} := \int_{-1}^{1} w(x)\,\bar{v}(x)\,dx\,.$$

This leads to an interesting side result concerning Legendre polynomials $P_n(x)$. Namely, having in mind the results on the spectral analysis for the operator K_0 (see Sect. 3.2 above) and applying Theorem 8 for $\varphi(x) \equiv 1$, we get

Corollary 2. *The Legendre polynomials $P_n(x)$ can be subsequently constructed as the functions $u_n(x)$, minimizing the functional*

$$\varkappa_0[u] := \int_{-1}^{1} \int_{-1}^{1} \frac{|u(x) - u(s)|^2}{|x - s|} \, dx \, ds \tag{64}$$

under the condition

$$u_n(x) \perp \bigvee_{l=0}^{n-1} u_l \,, \quad u_0(x) \equiv 1 \,, \tag{65}$$

where the orthogonality is with respect to the standard inner product in $L_2[-1,1]$.

We have completed the current discussion of 1D case and now turn to the higher dimensions.

4. Spectral estimations for the operators $\mathcal{K}_\varphi$ in higher dimensions

This section is devoted to the recently developed [13, 14, 15] generalization to the higher dimensions $M \geq 2$. Let us make the following important remark [13]:

Remark 6. (Representation of the operator $\mathcal{K}_\varphi$ in $\mathbb{R}^M$, $M \geq 2$)

Contrary to the 1D case, for any $M \geq 2$ the operator (1) can be represented as the sum of the integral operator and the operator of the multiplication by the function. Indeed, for $M \geq 2$ the integrand contains the weak (integrable) singularity $|\mathbf{x} - \mathbf{s}|^{-1}$ at $\mathbf{x} = \mathbf{s}$, so one can rewrite the representation (1) as

$$\mathcal{K}_\varphi : u(\mathbf{x}) \mapsto \varphi(\mathbf{x}) \int_{\mathbb{R}^M} \frac{u(\mathbf{s})}{|\mathbf{x} - \mathbf{s}|} \, d^M\mathbf{s} + W(\mathbf{x}) \, u(\mathbf{x}) \,, \tag{66}$$

where

$$W(\mathbf{x}) := - \int_{\mathbb{R}^M} \frac{\varphi(\mathbf{s})}{|\mathbf{x} - \mathbf{s}|} \, d^M\mathbf{s} \,. \tag{67}$$

Section 4 is organized as follows. In Sect. 4.1 we discuss the general issues for the spaces $\mathbb{R}^M$, $M \geq 2$, under some extra conditions for the functions $\varphi(\mathbf{x})$ and the domains $\operatorname{supp} \varphi = \Omega \subset \mathbb{R}^M$, and reduce the corresponding spectral problem to a countable set of 1D problems. Sect. 4.2 is devoted to the results on the spectral estimations obtained through the quadratic form approach. In Sects. 4.3 and 4.4 the specific systems in the most physically interesting cases $\mathbb{R}^2$ and $\mathbb{R}^3$ correspondingly are considered.

4.1. Dimensions $M \geq 2$: General scheme, completely admissible domains and reduction to a countable set of 1D problems

As described above in Sect. 1, the operators $\mathcal{K}_\varphi$ allow for the physical interpretation as the operators underlying the processes of the matter relaxation in the attractive field $\varphi(\mathbf{x}) \geq 0$ [13]. We assume that $\varphi(\mathbf{x})$ is an acceptable function in the sense od Definition 1 and its support $\Omega \subset \mathbb{R}^M$ is an admissible domain in the sense of

Definition 3. For the restricted to the subspace $L_2(\Omega)$ operators K_φ, following the representation (32) we have $K_\varphi = \varphi \circ K_0 - (K_0\varphi)$ and $Q_\varphi := \frac{1}{2\varphi} \circ K_\varphi = K_0 - V_\varphi$, where the reference operator K_0 corresponds to the homogeneous function $\varphi(\mathbf{x}) \equiv 1$, $\mathbf{x} \in \Omega$, and $V_\varphi(\mathbf{x}) := (K_0\varphi)(\mathbf{x})/(2\varphi(\mathbf{x}))$.

However, for $M \geq 2$, in general case, complete results in the spectral analysis of the generalized reference operators K_0 are not known [13] (contrary to 1D case – see Sect. 3.2 above), which prevents the application of the direct methods used in Sect. 3.3 for the analysis of the operators K_φ. Moreover, the calculations similar to ones shown under Sect. 3.5 for the quadratic form $\varkappa_\varphi[u]$ are not obvious.

Still, some results in this direction can be obtained under specific conditions discussed below [13]. Namely, let us define the so-called *completely admissible domains*:

Definition 4. *Compact convex domain* $\Omega \subset \mathbb{R}^M$, $M = N+1 \geq 2$, *is called as the completely admissible domain (or the pseudo-torus) if one can represent* Ω *as*

$$\Omega = \widehat{\mathbf{T}}^N := [0,R) \times \underbrace{\mathbf{C}^1 \times \mathbf{C}^1 \times \cdots \times \mathbf{C}^1}_{N\,\text{times}}, \tag{68}$$

where $\mathbf{C}^1$ *denotes a 1D circle. This means that every point* $\mathbf{x} \in \Omega$ *can be represented as*

$$\mathbf{x} = \{r, \boldsymbol{\Theta}\}, \tag{69}$$

where $r \in [0,R)$ *and* $\boldsymbol{\Theta} := (\theta_1, \theta_2, \ldots, \theta_N)$, $\theta_k \in [0, 2\pi)$, *are called as the pseudo-toroidal coordinates.*

Note that in dimension $M = 2$ (i.e., for $N = 1$) the pseudo-torus is a ring $\widehat{\mathbf{T}}^1 = \{\mathbf{x} : L_0 < |\mathbf{x}| < L\}$, $r = R(L - L_0)^{-1}(|\mathbf{x}| - L_0)$. In the degenerated case $L_0 = 0$ that is the disk $\widehat{\mathbf{T}}^1_{\text{deg}} = \{\mathbf{x} : 0 \leq |\mathbf{x}| < R\}$, $r = |\mathbf{x}|$. In dimension $M = 3$ (i.e., for $N = 2$) the pseudo-torus becomes the torus $\widehat{\mathbf{T}}^2 = \mathbf{T}^2$ with the big radius L and the small radius $R = L - L_0$. In the degenerated case $L_0 = 0$ the pseudo-torus $\widehat{\mathbf{T}}^2_{\text{deg}}$ is topologically equivalent to a 3D ball. These cases are considered in Sects. 4.2 and 4.3, respectively.

Further on in the present paper we restrict our consideration to the completely admissible domains in the sense of Definition 4, $\Omega = \widehat{\mathbf{T}}^N \subset \mathbb{R}^{N+1}$. In the pseudo-toroidal coordinates (69) the distance between two points $\mathbf{x} = \{r, \boldsymbol{\Theta}\}$, $\mathbf{s} = \{\rho, \boldsymbol{\Theta}'\} \in \widehat{\mathbf{T}}^N$ is

$$|\mathbf{x} - \mathbf{s}| = \Big[N(r^2 + \rho^2) - 2\,r\,\rho \sum_{l=1}^{N} \cos(\theta'_l - \theta_l)\Big]^{1/2}. \tag{70}$$

The measure $d^{N+1}\mathbf{x}$ in terms of the pseudo-toroidal coordinates $\mathbf{x} = \{r, \boldsymbol{\Theta}\}$ is

$$d^{N+1}\mathbf{x} = r^N\, dr\, d\theta_1\, d\theta_2 \cdots d\theta_N\,. \tag{71}$$

As the system of functions $\left\{e^{ik\theta}\right\}_{k\in\mathbb{Z}}$ forms an orthonormal basis in the space $L_2(\mathbf{C}^1)$, the system of functions $\left\{\exp\{i\mathbf{k\Theta}\}\right\}_{\mathbf{k}\in\mathbb{Z}^N}$, where

$$\exp\{i\mathbf{k\Theta}\} := \prod_{l=1}^{N} e^{ik_l\theta_l}\,, \tag{72}$$

forms an orthonormal basis in the space $L_2(\mathbf{C}^1 \times \mathbf{C}^1 \times \cdots \times \mathbf{C}^1)$. Therefore any function $u(\mathbf{x}) \in L_2(\widehat{\mathbf{T}}^N)$, $\mathbf{x} = \{r, \mathbf{\Theta}\}$, can be decomposed as

$$u(\mathbf{x}) = \sum_{\mathbf{k}\in\mathbb{Z}^N} u^{[\mathbf{k}]}(r)\,\exp\{i\mathbf{k\Theta}\}\,. \tag{73}$$

Let us assume that the field $\varphi(\mathbf{x})$ is pseudo-toroidaly symmetric, i.e., $\varphi(\mathbf{x}) = \varphi(r)$. Then the following statement is true (see [13], Theorem 4).

Theorem 9. *For any acceptable* (*in the sense of Definition* 1) *pseudo-toroidal symmetric function* $\varphi(\mathbf{x}) = \varphi(r)$ *having the completely admissible support* (*in the sense of Definition* 4) $\Omega \subset \mathbb{R}^M$, $M = N+1 \geq 2$, *i.e., the pseudo torus* $\Omega = \widehat{\mathbf{T}}^N$, *the subspaces*

$$\mathcal{H}^{[\mathbf{k}]} := \left\{u(\mathbf{x}) \in L_2(\Omega) :\, u(\mathbf{x}) = u^{[\mathbf{k}]}(r)\,\exp\{i\mathbf{k\Theta}\}\right\} \tag{74}$$

are invariant subspaces of the operator K_φ , *i.e.,*

$$K_\varphi :\, \mathcal{H}^{[\mathbf{k}]} \,\mapsto\, \mathcal{H}^{[\mathbf{k}]}\,, \tag{75}$$

for all $\mathbf{k} \in \mathbb{Z}^N$.

Proof. The claim was obtained in [13, Theorem 4] by straightforward calculation. In particular, it was shown in [13] that for any $u(\mathbf{x}) = u^{[\mathbf{k}]}(r)\,\exp\{i\mathbf{k\Theta}\} \,\in\, \mathcal{H}^{[\mathbf{k}]}$,

$$(K_\varphi u)(\mathbf{x}) = \exp\{i\mathbf{k\Theta}\}\, Y^{[\mathbf{k}]}_{N,R,\varphi}[u(r), r] \,\in\, \mathcal{H}^{[\mathbf{k}]}\,, \tag{76}$$

where

$$\begin{aligned} Y^{[\mathbf{k}]}_{N,R,\varphi}[u(r), r] \,:=\, & \int_0^R \rho^N \int_0^{2\pi}\!\!\cdots\!\int_0^{2\pi} \\ & \times\, \frac{u(r)\,\varphi(\rho) - u(\rho)\,\varphi(r)\,\prod_{l=1}^N \cos k_l\vartheta_l}{\left[N(r^2+\rho^2) - 2r\rho\sum_{m=1}^N \cos\vartheta_m\right]^{1/2}}\, d\rho\, d\vartheta_1\cdots d\vartheta_N\,. \end{aligned} \tag{77}$$

It is convenient to introduce functions

$$Z^{[\mathbf{k}]}_N(r,\rho) := \int_0^{2\pi}\!\!\cdots\!\int_0^{2\pi} \frac{\prod_{l=1}^N \cos k_l\vartheta_l}{\left[N(r^2+\rho^2) - 2r\rho\sum_{m=1}^N \cos\vartheta_m\right]^{1/2}}\, d\vartheta_1\cdots d\vartheta_N\,. \tag{78}$$

Then the formula (77) can be written as

$$Y^{[\mathbf{k}]}_{N,R,\varphi}[u(r), r] := \int_0^R \rho^N\, \left[u(r)\,\varphi(\rho)\, Z^{[\mathbf{0}]}_N(r,\rho) - u(\rho)\,\varphi(r)\, Z^{[\mathbf{k}]}_N(r,\rho)\right] d\rho\,. \tag{79}$$

In a sense, the functions $Z_N^{[\mathbf{k}]}(r,\rho)$, having a weak (integrable) singularity at $r=\rho$ play for the operator K_φ in the $(N+1)$-dimensional case the role similar to the singular (but non-integrable) function $|x-s|^{-1}$ in the 1D case. □

Theorem 9 implies the following

Corollary 3. *Under the conditions of Theorem 9 the operators K_φ and Q_φ can be decomposed into the orthogonal sums of partial operators,*

$$K_\varphi = \sum_{\mathbf{k}\in\mathbb{Z}^N} \oplus K_\varphi^{[\mathbf{k}]}\,, \quad Q_\varphi = \sum_{\mathbf{k}\in\mathbb{Z}^N} \oplus Q_\varphi^{[\mathbf{k}]}\,, \tag{80}$$

where the partial operators $K_\varphi^{[\mathbf{k}]}$ and $Q_\varphi^{[\mathbf{k}]}$ act in the Hilbert space $\mathcal{H}^{[0]}$ as

$$K_\varphi^{[\mathbf{k}]} : u(r) \mapsto Y_{N,R,\varphi}^{[\mathbf{k}]}[u(r),r]\,, \quad Q_\varphi^{[\mathbf{k}]} : u(r) \mapsto \frac{1}{2\varphi(r)}\, Y_{N,R,\varphi}^{[\mathbf{k}]}[u(r),r]\,. \tag{81}$$

Corollary 3 allows reducing the spectral problems for the operators K_φ and Q_φ to the countable sets of the 1D problems for the partial operators $K_\varphi^{[\mathbf{k}]}$ and $Q_\varphi^{[\mathbf{k}]}$. That is the subject of the next Subsection.

4.2. Spectral estimations for the operators $\mathcal{K}_\varphi$ and $\mathcal{Q}_\varphi$, corresponding to an acceptable pseudo-toroidal symmetric functions $\varphi(r)$ having completely admissible support $\Omega = \widehat{\mathbf{T}}^N \subset \mathbb{R}^M$

The results described in Sect. 4.1 above give a hint to obtain the spectral estimations for the operators $\mathcal{K}_\varphi$ and $\mathcal{Q}_\varphi$ similarly to 1D case discussed above in Sect. 3.5. To do it, we again use the quadratic form approach and further comparison with the generalized reference operator $\mathcal{K}_0$, corresponding to the homogeneous field $\varphi(\mathbf{x}) \equiv 1$ in the domain $\Omega = \widehat{\mathbf{T}}^N$ and $\varphi(\mathbf{x}) \equiv 0$ outside the domain Ω.

Although the exact solution of the spectral problem for the restricted operator K_0 in the $(N+1)$-dimensional case is not known, we can provide some spectral estimations. Due to Corollary 4, the spectrum of the restricted reference operator K_0 is the union of the spectra of the partial operators,

$$\sigma(K_0) = \bigcup_{\mathbf{k}\in\mathbb{Z}^N} \sigma(K_\varphi^{[\mathbf{k}]})\,. \tag{82}$$

Using the formulae (76), (78), (79) for $\varphi(r) \equiv 1$ at $r \in [0,R)$, and the obvious property $Z_N^{[\mathbf{k}]}(r,\rho) = Z_N^{[\mathbf{k}]}(\rho,r)$, in [13] it was shown that the quadratic form of the reference partial operator $K_0^{[\mathbf{k}]} = 2Q_0^{[\mathbf{k}]}$ in the appropriate Hilbert space $L_2([0,R];\, r^N dr)$ is

$$\begin{aligned}\varkappa_0^{[\mathbf{k}]}[u] &:= \langle (K_0^{[\mathbf{k}]}u), u\rangle_{L_2([0,R];\, r^N dr)} \\ &= \iint_\Delta dr\, d\rho \left\{ \Big[|u(r)|^2 + |u(\rho)|^2\Big]\, Z_N^{[\mathbf{0}]}(r,\rho) \right. \\ &\qquad\qquad \left. -\ \Big[u(\rho)\,\bar u(r) + u(r)\,\bar u(\rho)\Big]\, Z_N^{[\mathbf{k}]}(r,\rho) \right\} \\ &= \mathcal{I}_1[u] + \mathcal{I}_2[u],\end{aligned} \tag{83}$$

where we integrate over the triangle $\Delta = \{(r,\rho) : 0 \le \rho \le r \le R\} \subset \mathbb{R}^2$. Here

$$\mathcal{I}_1^{0;\,[\mathbf{k}]}[u] := \iint_\Delta dr\, d\rho \left[|u(r) - u(\rho)|^2\right] Z_N^{[\mathbf{k}]}(r,\rho) \tag{84}$$

and

$$\mathcal{I}_2^{0;\,[\mathbf{k}]}[u] := \iint_\Delta dr\, d\rho \left[|u(r)|^2 + |u(\rho)|^2\right] \left(Z_N^{[\mathbf{0}]}(r,\rho) - Z_N^{[\mathbf{k}]}(r,\rho) \right). \tag{85}$$

This allows for the following generalization of Theorem 6.

Theorem 10. *For any acceptable function* $\varphi(\mathbf{x}) = \varphi(r)$ *with completely admissible support* $\operatorname{supp}\varphi = \mathbf{T}^N$*, the quadratic forms* $\varkappa_\varphi^{[\mathbf{k}]}[u]$ *of the operators* $Q_\varphi^{[\mathbf{k}]}$, $\mathbf{k} \in \mathbb{Z}^N$ *are nonnegative,* $\varkappa_\varphi^{[\mathbf{k}]}[u] \ge 0$*, and has the sharp lower boundary* $m_\varphi^{[\mathbf{k}]} := \min_u \varkappa_\varphi^{[\mathbf{k}]}[u]$*, achieved with* $u(\mathbf{x}) \equiv \varphi(r) : \varkappa_\varphi^{[\mathbf{k}]}[\varphi] = 0$.

This theorem was proved in [13] (see Theorem 1 there) through the exploitation of the results shown for the 1D case in Sect. 3.5.

Remark 7. (Attractive and repulsive external fields φ)

Proved non-negativity of the operators $Q_\varphi^{[\mathbf{k}]}$ for non-negative (attractive) acceptable toroidal-symmetric fields $\varphi(r)$ means the exponential extinction of the upper modes ($\mathbf{k} \ne 0$) in time with the Lyapunov coefficients $\nu_n^{[\mathbf{k}]}$. Physically, this corresponds to the relaxation of the system to an equilibrium state. Contrary, if the field $\varphi(r)$ is repulsive (change $\varphi(r) \to -\varphi(r)$), the eigenvalues $\nu_n^{[\mathbf{k}]}$ also change their sign, so the upper modes increase in time and one will observe a chaotic evolution of the system. Mixed case ($\varphi(r)$ is not of a certain sign) demands the separate investigation.

Using the representation (83), one can consider the spectral estimation for the operator $Q_\varphi^{[\mathbf{k}]}$ from above. This was done in [13] through the linear change of variables variables $x = 2r/R - 1$, which maps the interval $[0,R]$ onto $[-1,1]$. The quadratic form $\varkappa_0^{[\mathbf{k}]}[u]$ can be estimated [13] as

$$\varkappa_0^{[\mathbf{k}]}[u] = \mathcal{I}_1^{0;\,[\mathbf{k}]}[u] + \mathcal{I}_2^{0;\,[\mathbf{k}]}[u]\,,$$

where

$$\mathcal{I}_1^{0;\,[\mathbf{k}]}[u] \le (2\,\pi)^{N/2}\,R^{2N-1}\,\varkappa_0^{[\mathbf{k}]}[u]\,; \quad \mathcal{I}_2^{0;\,[\mathbf{k}]}[u] \le 2\,\sqrt{2}\,(2\,\pi)^{N/2}\,\mathcal{B}_N^{[\mathbf{k}]}\,R\,||u||_0^2\,.$$

Here

$$||u||_0^2 := \int_0^R r^N\,|u(r)|^2\,dr$$

and

$$\mathcal{B}_N^{[\mathbf{k}]} := \int_0^\pi \ldots \int \frac{1-\prod_{l=1}^N \cos k_l\theta_l}{\left[N^{-1}\,\sum_{m=1}^N (1 = \cos\theta_m\right]^{1/2}}\,d\theta_1\cdots d\theta_N \;<\; \infty$$

for all $\mathbf{k} \in \mathbb{Z}^N$. Therefore,

$$\varkappa_0^{[\mathbf{k}]}[u] \le \mathcal{A}_1(N,R)\,\varkappa_0[u] + \mathcal{A}_2^{[\mathbf{k}]}(N,R)\,||u||_0^2\,, \tag{86}$$

where

$$\mathcal{A}_1(N,R) := (2\,\pi)^{N/2}\,R^{2N}\,, \quad \mathcal{A}_2(N,R) := 4\,\sqrt{2}\,(2\,\pi)^{N/2}\,\mathcal{B}_N^{[\mathbf{k}]}\,R\,.$$

With the minimal principle for the quadratic forms [1] this estimation leads [13] to

Lemma 3. *The discrete spectrum of the reference operator K_0 acting in the Hilbert space $L_2(\mathbf{T}^N;\, r^N\,dr)$ is formed by the countable set*

$$\sigma_d(K_0) = \left\{\mu_n^{[\mathbf{k}]}\right\}_{n\in\mathbb{Z}}^{\mathbf{k}\in\mathbb{Z}^N} \tag{87}$$

where $\mu_n^{[\mathbf{k}]}$ are the eigenvalues of the partial operators $K_0^{[\mathbf{k}]}$ and are estimated as

$$\mu_n^{[\mathbf{k}]} \le \mathcal{A}_1(N,R)\,\mu_n + \mathcal{A}_2(N,R)\,. \tag{88}$$

In order to get similar spectral estimations for the operator Q_φ, corresponding to an arbitrary pseudo-toroidal symmetric acceptable function $\varphi(\mathbf{x}) = \varphi(r)$, in [13] the following estimation was obtained for the effective potential $V_\varphi(r)$:

$$|(V_\varphi\,u\,,\,u)| \le \mathcal{A}_3(N,R;\varphi)\,||u||_0^2\,, \tag{89}$$

where

$$\mathcal{A}_3(N,R;\varphi) := (2\pi)^{N/2}\,R^N\,A_\varphi\,\varepsilon_\varphi^{-2}\,.$$

Representation [13]

$$(V_\varphi\,u\,,\,u) = \iint_\Delta (\rho\,r)^N\,Z_N^{[\mathbf{0}]}\left[\big(1-\varphi(\rho)/\varphi(r)\big)\,|u(r)|^2 + \big(1-\varphi(r)/\varphi(\rho)\big)\,|u(\rho)|^2\right]d\rho\,dr \tag{90}$$

together with Corollary 3, Lemma 3, estimate (90), and minimal principle for quadratic forms [1] lead to the following statement (see [13], Theorem 6):

Theorem 11. *For any acceptable pseudo-toroidal symmetric function $\varphi(r)$, the discrete spectrum of the corresponding operator Q_φ is formed by the countable set*

$$\sigma_d(Q_\varphi) = \{\nu_n^{[\mathbf{k}]\,\varphi}\}_{n\in\mathbb{Z}_+}^{\mathbf{k}\in\mathbb{Z}^N}\,, \tag{91}$$

where $\nu_n^{[\mathbf{k}],\varphi}$ *are the eigenvalues of the partial operator* $Q_\varphi^{[\mathbf{k}]}$ *and are estimated as*

$$\frac{1}{2}\,\mu_n^{[\mathbf{k}]} - \mathcal{A}_3(N,R;\varphi) \le \nu_n^{[\mathbf{k}]\,\varphi} \le \frac{1}{2}\,\mu_n^{[\mathbf{k}]} + \mathcal{A}_3(N,R;\varphi)\,, \tag{92}$$

which implies their estimation from above as

$$\nu_n^{[\mathbf{k}]\,\varphi} \le \mathcal{A}_1(N,R)\,\mu_n^{[\mathbf{k}]} + \mathcal{A}_2^{[\mathbf{k}]}(N,R) + \mathcal{A}_3(N,R;\varphi)\,. \tag{93}$$

Due to condition (5), we immediately have a similar spectral estimation for the operators $K_\varphi = 2\varphi \circ Q_\varphi$:

Corollary 4. *For any acceptable pseudo-toroidal symmetric function* $\varphi(r)$*, the discrete spectrum of the corresponding operator* K_φ *is formed by the countable set*

$$\sigma_d(K_\varphi) \,=\, \big\{\tau_n^{[\mathbf{k}],\,\varphi}\big\}_{n\in\mathbb{Z}_+}^{\mathbf{k}\in\mathbb{Z}^N}\,, \tag{94}$$

where $\tau_n^{[\mathbf{k}],\varphi}$ *are the eigenvalues of the partial operator* $K_\varphi^{[\mathbf{k}]}$ *and are estimated as*

$$RA_\varphi\,\mu_n^{[\mathbf{k}]} - 2RA_\varphi\mathcal{A}_3(N,R;\varphi) \le \tau_n^{[\mathbf{k}],\,\varphi} \le RA_\varphi\,\mu_n^{[\mathbf{k}]} + 2RA_\varphi\mathcal{A}_3(N,R;\varphi))\,, \tag{95}$$

which implies their estimate from above as

$$\tau_n^{[\mathbf{k}],\,\varphi} \le 2R\big[\mathcal{A}_1(N,R)\,\mu_n^{[\mathbf{k}]} + \mathcal{A}_2^{[\mathbf{k}]}(N,R) + \mathcal{A}_3(N,R;\varphi)\big]\,. \tag{96}$$

Corollary 4 means that under the conditions of Theorem 11, the discrete spectrum $\sigma_d(K_\varphi)$ is formed by infinite countable sets of the eigenvalues of the partial operators $K_\varphi^{[\mathbf{k}]}$. They are numerated by multi-index $\mathbf{k} \in \mathbb{Z}^N$ and index $n = 0,1,2,\ldots$ The asymptotics of these eigenvalues with respect to the index $n \to \infty$ is determined by the corresponding asymptotics of $\mu_n = 2\sum_{j=1}^{n} 1/j$, which is logarithmic [34]: $\mu_n = 2\left[\mathbf{C}+\ln n+(2n)^{-1}\right] + o(n^{-1})$, where $\mathbf{C} = 0.577\ldots$ is the Euler constant.

Using the results shown above, in [13] Theorem 8 was generalized to higher dimensions as follows

Theorem 12. *For any acceptable pseudo-toroidal symmetric function* $\varphi(r)$*, the eigenfunctions* $u_n^{[\mathbf{k}],\varphi}(r)$ *and the eigenvalues* $\nu_n^{[\mathbf{k}],\varphi}$ *can be find through the minimization of the functional*

$$\begin{aligned}\varkappa_\varphi[u] = \int_0^R\!\!\int_0^R (r\,\rho)^N \Bigg\{ &|u(r)-u(\rho)|^2\, Z_N^{[\mathbf{k}]}(r,\rho) + \Big[|u(r|^2+|u\rho)|^2\Big]\,\Big[Z_N^{[\mathbf{0}]}(r,\rho) \\ &- Z_N^{[\mathbf{k}]}(r,\rho)\Big] - 2\,\frac{\varphi(r)-\varphi(\rho)}{\varphi(r)\,\varphi(\rho)}\,\Big[|u(r|^2-|u\rho)|^2\Big]\Bigg\}\,dr\,d\rho\end{aligned} \tag{97}$$

under the condition

$$u_n^{[\mathbf{k}],\,\varphi}(r) \;\perp\; \bigvee_{l=0}^{n-1}\,; \qquad u_n^{[\mathbf{k}](r),\,\varphi} \equiv\; \delta_{k_1 0}\,\delta_{k_2 0}\cdots\delta_{k_N 0}\,\varphi(r)\,. \tag{98}$$

Here the functions $Z_N^{[\mathbf{k}]}(r,\rho)$ *are defined by formula* (78)*.*

Remark 8. (Special functions generated by $Z_N^{[\mathbf{k}]}(r,\rho)$)

The kernels $Z_N^{[\mathbf{k}]}(r,\rho)$ generate special functions $\Xi_N^{[\mathbf{k}]}(z)$ defined as

$$\Xi_N^{[\mathbf{k}]}(x) = \frac{1}{2\,\pi^{N/2}}\, Z_N^{[\mathbf{k}]}(r, r\,x)\,. \tag{99}$$

The functions $\Xi_N^{[\mathbf{k}]}(z)$ were introduced in [13] and further investigated in [28] (for $N = 1$) and [30] (for $N = 1$ and $N = 2$). The key results are outlined below in Sect. 5 of the present paper.

Now let us address the results obtained for the specific 2D and 3D domains Ω in [14] and [15], respectively.

4.3. Planar case and application to the thin film relaxation processes

In [14] the above described technique was applied to the specific case of an acceptable external field $\varphi(\mathbf{x})$ having the completely accessible planar support $\Omega_R := \widehat{\mathbf{T}}^2_{\text{deg}} \subset \mathbb{R}^2$, which is the disc

$$\Omega_R = \widehat{\mathbf{T}}^2_{\text{deg}} = \{\mathbf{x} \in \mathbb{R}^2 : |\mathbf{x}| < R\}$$

of radius R. The operator $\mathcal{K}_\varphi$ determines the dynamics of the thin film relaxation in the external attractive field $\varphi(\mathbf{x}) \geq 0$ through the dynamical equation (3).

We restrict our consideration here to the circular symmetric fields $\varphi(\mathbf{x}) = \varphi(r)$, $r := |\mathbf{x}| \in [0, R)$. The function $q_\varphi(\mathbf{x}) := \int_0^R \varphi(\mathbf{x})\, |\mathbf{x}-\mathbf{s}|^{-1}\, d^2\mathbf{s}$ then equals

$$q_\varphi(\mathbf{x}) = q_\varphi(r) = \int_0^{2\pi} d\vartheta \int_0^\rho \frac{\varphi(\rho)\, d\rho}{[1 + y^2 - 2y\cos\vartheta]^{1/2}}\,. \tag{100}$$

One can see that $q_\varphi(r) \to 0$ at $r \to \infty$ and

$$q_\varphi(\mathbf{x}) \leq M_{\varphi,R} := \max_{\rho\in[0,R]} \varphi(\rho) \int_{\Omega_R} |\mathbf{x}-\mathbf{s}|^{-1}\, d^2\mathbf{s} \leq \varepsilon_\varphi + 2RA_\varphi\,. \tag{101}$$

To estimate the upper boundary, let us consider a point $\mathbf{x} \to \partial\Omega$. As $\varphi(\mathbf{x})$ is an acceptable function in the sense of Definition 1, obviously

$$\max_{\rho\in[0,R]} \varphi(\rho) \leq \varepsilon_\varphi + 2RA_\varphi\,.$$

We introduce a disc $\mathbf{C}_\omega(\mathbf{x}) \subset \mathbb{R}^2$ of radius ω with the center in the point $\mathbf{x}$. We decompose the domain of integration Ω_R in formula (100) into two domains $\Omega^\omega_{R,1} := \Omega_R \cap \mathbf{C}_\omega(\mathbf{x})$ and $\Omega^\omega_{R,2} := \Omega_R \backslash \Omega^\omega_{R,1}$. Estimating the integrals over $\Omega^\omega_{R,1}$ and $\Omega^\omega_{R,2}$ separately, one gets [28]

$$q_\varphi(\mathbf{s}) \leq \omega^{-1} + \omega\,(\varepsilon_\varphi + 2RA_\varphi)\,. \tag{102}$$

As the parameter $\omega > 0$ is a subject of our choice, in order to minimize the right-hand side of the inequality (102), we take it as $\omega = (\varepsilon_\varphi + 2RA_\varphi)^{-1/2}$ and get

$$q_\varphi(\mathbf{s}) \leq 2\,(\varepsilon_\varphi + 2RA_\varphi)^{1/2}\,. \tag{103}$$

Therefore, contrary to 1D case, here the absolute continuous spectrum of the operator $\mathcal{K}_\varphi$ generated by the function $q_\varphi(\mathbf{x})$ is bounded from above,

$$\sigma_{ac}(\mathcal{K}_\varphi) \subseteq [0, M_{\varphi,R}]\,; \quad M_{\varphi,R} \le (\varepsilon_\varphi + 2RA_\varphi)^{1/2}\,. \tag{104}$$

We can get the precise expression for the value $M_{\varphi,R}$. The equality (100) can be written [28] terms of the complete elliptic integral of the first kind $\mathbf{K}(p)$ [34, 35, 36] as

$$q_\varphi(r) = 4\,r^2 \int_0^1 \frac{y\,\varphi(ry)}{[1+y^2]^{1/2}}\,\frac{1-y}{1+y}\,\mathbf{K}\Big(\frac{2\,y^{1/2}}{1+y}\Big)\,dy\,, \tag{105}$$

where $r > R \ge \rho$. Hence

$$M_{\varphi,R} = \lim_{r\to R+0} q_\varphi(r) = 4\,R^2 \int_0^1 \frac{y\,\varphi(Ry)}{[1+y^2]^{1/2}}\,\frac{1-y}{1+y}\,\mathbf{K}\Big(\frac{2\,y^{1/2}}{1+y}\Big)\,dy \,<\, \infty\,. \tag{106}$$

The absolute continuous spectrum of the operator $\mathcal{K}_\varphi$ generated by the function $q_\varphi(\mathbf{x})$ has infinite countable multiplicity in the interval $[0, M_{\varphi,R}]$, as the similar to formula (106) estimates are valid for all partial operators $\mathcal{K}_\varphi^{[k]}$, $k \in \mathbb{Z}$. Indeed, the system under discussion in this Subsection is a particular case of the systems discussed above in Sect. 4.2. Therefore, the operator $\mathcal{K}_\varphi$ can be presented as the orthogonal series of the partial operators, $\mathcal{K}_\varphi = \sum_{k\in\mathbb{Z}} \oplus\, \mathcal{K}_\varphi^{[k]}$. Note that the operators $\mathcal{K}_\varphi^{[k]}$ coincide for $\pm k$. This implies

$$\sigma(\mathcal{K}_\varphi) = \overline{\bigcup_{k\in\mathbb{Z}_+} \sigma(\mathcal{K}_\varphi^{[k]})}\,. \tag{107}$$

All the partial operators $q_\varphi^{[k]}$ act as the operators of the multiplication by the same function $q_\varphi(r)$ given by the formula (105).

Recalling the results of Sect. 4.2, for the planar system discussed here one gets [28] the following spectral estimate for eigenvalues $\tau_n^{[k],\,\varphi}$ of the partial restricted operators $K_\varphi^{[k]}$:

$$\widehat{\mu_n^{[k]}} \;-\pi\,R^2\,A_\varphi^2\,\varepsilon_\varphi^{-2} \le \tau_n^{[k],\,\varphi} \le \widehat{\mu}_n^{[k]} \;+\pi\,R^2\,A_\varphi^2\,\varepsilon_\varphi^{-2}\,, \tag{108}$$

where $n, k \in \mathbb{Z}_+$;

$$0 \le \widehat{\mu}_n^{[k]} \le \pi\,R\,(R\,\mu_n + 4\,\sqrt{2}\,\mathcal{N}^{[k]})\,; \tag{109}$$

$$\mathcal{N}^{[k]} := \int_0^\pi \frac{1-\cos k\theta}{\sqrt{1-\cos\theta}}\,d\theta\,.$$

In particular, as $\mathcal{N}^{[0]} = 0$, one gets

$$-\,\pi\,R^2\,A_\varphi^2\,\varepsilon_\varphi^{-2} \le \tau_n^{[0],\,\varphi} \le \pi\,R^2\,\mu_n + A_\varphi^2\,\varepsilon_\varphi^{-2}\,.$$

Let us show an example of the absolutely continuous spectrum similar to Examples 1–3 above.

Example 4. (A brunch of absolutely continuous spectrum parametrically going to $\mathbb{R}_+$)

As discussed above, the absolutely continuous spectrum of the operator $\mathcal{K}_\varphi$ is generated by the image of the function $q_\varphi(\mathbf{x}) = \int_{\mathbb{R}^M} \varphi(\mathbf{x})|\mathbf{x}-\mathbf{s}|^{-1} d^M\mathbf{s}$. Therefore, one can design function $q_\varphi(\mathbf{x})$ with desirable properties and then reconstruct function $\varphi(\mathbf{x})$ inverting the Riesz potential. In case $M = 2$ the inversion looks like (see, e.g., [42, 43]):

$$\varphi(\mathbf{x}) = \frac{1}{\pi} \lim_{\epsilon\to 0} \epsilon^{-2} \int_{\mathbf{R}^2} F(3/2, 2; 1; -|\mathbf{y}|^2)\, q_\varphi(\mathbf{x}-\epsilon\mathbf{y})\, d^2\mathbf{y}\,,$$

where F stands for the Gauss hypergeometric function [33]. Taking, e.g., $q_\varphi(\mathbf{x}) = a\, e^{-a\mathbf{x}}$ we get its image equal $(0, a)$ in $\mathbb{R}^2$, which generates the absolutely continuous spectrum of infinite multiplicity coinciding with interval $(0, a)$ and thus going to $\mathbb{R}_+$ when $a \to +\infty$.

Now we consider a specific relaxation process.

Example 5. (Relaxation process in a plane for dotted-inserted matter)

Let us illustrate the above discussion with the most simple example of the relaxation of dotted-inserted matter in the homogeneous center-symmetric field

$$\varphi(\mathbf{x}) = \chi_R(\mathbf{x}) \tag{110}$$

where $\chi_R(\mathbf{x})$ stands for the characteristic function of the disk Ω_R, i.e. here the dynamics is determined by the reference operator $\mathcal{K}_0$. We assume that in the past $(t < 0)$ there was no matter in the system, i.e., $U(\mathbf{x}; t) \equiv 0$ at $t < 0$. Then, at the time moment $t = 0$ one had perturbed the system by dotted adding a portion of matter in a point $\mathbf{p} \in \mathbb{R}^2\backslash\Omega_R$, so

$$U(\mathbf{x}; 0) = \delta(\mathbf{x}-\mathbf{p})\,. \tag{111}$$

We consider the evolution of the system (i.e., the perturbation relaxation) under the dynamical law (2) in the homogeneous field (110) with initial condition (111). In this case, obviously $\varepsilon_0 = 1$ and $A_0 = 0$, so according to formula (104) we have $M_{\chi,R} \le 1$.

We use the basis formed by the (generalized) eigenfunctions of the operator $\mathcal{K}_0$ to decompose function $U(\mathbf{x}; 0)$ with its (generalized) eigenfunctions. This decomposition looks like

$$U(\mathbf{x}; 0) = \sum_{k\in\mathbb{Z}} \left(\sum_{n\ge 0} \zeta_n^{[k]}\, u_n^{[k,\,0]}(\mathbf{x}) + \int_0^1 \zeta_\nu^{[k]}\, u_\nu^{[k,\,0]}(\mathbf{x})\, d\nu \right), \tag{112}$$

where $u_n^{[k]}(\mathbf{x}) = e^{i;k\theta} u_n^{[k]}(r)$ are the eigenfunctions and $u_\nu^{[k]}(\mathbf{x}) = e^{ik\theta} u_\nu^{[k]}(r)$ are the generalized eigenfunctions of the partial operators $K_0^{[k]}$ corresponding to the eigenvalues $\tau_n^{[k\ 0]}$ and the points of the absolutely continuous spectrum $\nu \in \sigma_{ac}(K_0^{[k]})$

respectively. The decomposition coefficients are calculated as the inner products in the Hilbert space $L_2(\mathbb{R}^2)$:

$$\zeta_n^{[k]} = \int_{\mathbb{R}^2} U(\mathbf{s})\,\bar{u}_n^{[k,\,0]}(\mathbf{s})\,d^2\mathbf{s} = \frac{1}{q_0(\mathbf{p}) - \tau_n^{[k\ 0]}} \int_{\mathbb{R}^2} \frac{u_n^{[k,\,\bar{0}]}(\mathbf{s})}{|\mathbf{p}-\mathbf{s}|}\,d^2\mathbf{s}\,; \tag{113}$$

$$\zeta_\nu^{[k]} = \int_{\mathbb{R}^2} U(\mathbf{s};0)\,\bar{u}_\nu^{[k,\,0]}(\mathbf{s})\,d^2\mathbf{s} = \delta(q_0(\mathbf{p}) - \nu)\,. \tag{114}$$

Therefore, the evolution in time of the system considered in this example is

$$U(x;t) = \sum_{k\in\mathbb{Z}}\sum_{n\geq 0} \zeta_n^{[k]}\,u_\nu^{[k,\,0]}(\mathbf{x})\,e^{-\tau_n^{[k\ 0]}t} + \delta(\mathbf{x}-\mathbf{p})\,e^{-q_0(\mathbf{p})t}\,. \tag{115}$$

Now let us turn to some specific 3D systems.

4.4. Application to the matter relaxation processes in cylindric 3D domains

We consider cylindric domain

$$\Omega_{R,H} = \{\mathbf{x} = (x_1, x_2, x_3) \in \mathbb{R}^3 : x_1^2 + x_2^2 < R^2, -H < x_3 < H\}$$

and introduce the cylindric coordinates

$$(r,\theta,h) :\ x_1 = r\cos\theta,\ x_2 = r\sin\theta,\ -H \leq h := x_3 \leq H,$$

where (x_1, x_2, x_3) are Cartesian coordinates in $\mathbb{R}^3$. In this case the upper boundary of the absolute continuous spectrum of the corresponding operator $\mathcal{K}_\varphi$ generated by the image of the function $q_\varphi(\mathbf{x})$ for any acceptable function $\varphi(\mathbf{x})$ with the support $\operatorname{supp}\varphi = \Omega_{R,H}$ (compare to (104) is estimated as (see [15, Theorem 1])

$$m_\varphi^{\Omega_{R,H}} \leq \frac{3}{2}\,(2\,\pi)^{1/3}\left(\varepsilon_\varphi + 2\,A_\varphi\sqrt{R^2+H^2}\right)^{1/3}.$$

In particular, for $\varphi(\mathbf{x}) = \chi_{\Omega_{R,H}}(\mathbf{x})$, $m_0^{\Omega_{R,H}} \leq \frac{3}{2}\,(2\,\pi)^{1/3}$.

Despite $\Omega_{R,H}$ is not a pseudo torus, for the functions $\varphi(\mathbf{x})$ having the specific symmetry, the partial analysis of the operators $\mathcal{K}_\varphi$ is possible and the corresponding spectral estimates can be obtained [15]. We assume that $\varphi(\mathbf{x})$ is an axial-symmetric and homogeneous with respect to the coordinate h function, i.e., $\varphi(\mathbf{x}) = \varphi(r)$. In this case [15] the operator $\mathcal{K}_\varphi$ is decomposed as

$$\mathcal{K}_\varphi = \sum_{l,n\in\mathbb{Z}} \oplus\,\mathcal{K}_\varphi^{[l,k]}\,,$$

where the partial operators $\mathcal{K}_\varphi^{[l,k]}$ act from $\mathcal{H}^{[l,k]} := \{u(\mathbf{x}) = e^{i\pi l h/H}\,e^{ik\theta}\,u(r)\}$ into $\mathcal{H}^{[l,k]}$ as

$$\mathcal{K}_\varphi^{[l,k]} :\ e^{i\pi l h/H}\,e^{ik\theta}\,u(r)\ \mapsto$$
$$e^{i\pi l h/H}\,e^{ik\theta}\,r \iint_{-H}^{H} dh \int_0^1 \Big[\Phi_{h/r}^{[0,0]}(y)\,u(r)\,\varphi(r\rho) - \Phi_{h/r}^{[l,k]}(y)\,u(r\rho)\,\varphi(r)\Big]\,dy\ .$$

Here

$$\Phi_g^{[l,k]}(y) := \int_0^{2\pi} \frac{\cos(\pi lrg/H)\,\cos(ik\theta)}{[1+y^2-2y\cos\theta+g^2]^{1/2}}\,d\theta\,.$$

One can note that the partial operators $\mathcal{K}_\varphi^{[l,k]}$ generate special functions

$$\Psi_g^{[k]}(z) := \int_0^{2\pi} \frac{\cos(ik\theta)}{[1+z^2-2z\cos\theta+g^2]^{1/2}}\,d\theta\,.$$

These functions are related to the functions $\Xi_1^{[k]}(z)$ defined by formula (99) and studied below in Sect. 5.2 as

$$\Psi_0^{[k]}(z) = \Xi_1^{[k]}(z)\,.$$

4.5. Application to the matter relaxation processes in and toroidal 3D domains

Now we will briefly mention the results [15] for 3D toroidal domains $\Omega = T_{R,Y} := \{\mathbf{x} = (r,\phi,\theta) : 0 \le r < R, 0 \le \phi < 2\pi, 0 \le \theta < 2\pi\}$, and Cartesian coordinates are $x_1 = r\cos\theta + y\cos\phi$, $x_2 = r\cos\theta + y\cos\phi$, $x_3 = r\sin\theta$; $0 \le y < Y$. We assume that $\varphi(\mathbf{x})$ is a so called biangular-symmetric function, i.e., symmetric with respect to the angular coordinates ϕ and θ: $\varphi(\mathbf{x}) = \varphi(r)$. We also assume that the matter flow cannot penetrate through the surface of domain $\Omega = T_{R,Y}$ and that $L \ll R$. In this case the physical distance $|\mathbf{x}-\mathbf{s}|$ between points $\mathbf{x} = (r,\phi,\theta)$ and $\mathbf{s} = (\rho,\phi',\theta')$ in $\Omega = T_{R,Y}$ is naturally replaced by

$$\Delta(\mathbf{x},\mathbf{s}) := \kappa(|\theta-\theta'|) + \Big[r^2+\rho^2-2\,r\,\rho\,\cos(\phi-\phi')\Big]^{-1/2}, \qquad (116)$$

where

$$\kappa(\alpha) := \begin{cases} \alpha\,, & \text{if } 0 \le \alpha \le \pi\,; \\ 2\,\pi-\alpha\,, & \text{if } \pi \le \alpha \le 2\,\pi\,. \end{cases}$$

So, we consider the operator

$$\widetilde{\mathcal{K}}_\varphi : u(\mathbf{x}) \mapsto \int_{\mathbb{R}^3} \frac{\big(u(\mathbf{x}\,\varphi(\mathbf{s}) - u(\mathbf{s}\,\varphi(\mathbf{x})\,(\mathbf{x},\mathbf{s})\big)}{\Delta(\mathbf{x},\mathbf{s})}\,d^3\mathbf{s}\,. \qquad (117)$$

In this case the following statements are valid (see [15]: Theorem 3, Lemma 1, Lemma 2 and Theorem 4).

Theorem 13. *For any acceptable biangular-symmetric field $\varphi(\mathbf{x}) = \varphi(r)$ having the toroidal support* $\operatorname{supp}\varphi = T_{R,Y}$*, the subspaces*

$$\mathcal{H}^{[l;m]} := \big\{u(\mathbf{x}) \in L_2(\mathbb{R}^3 : u(\mathbf{x}) := e^{il\theta}\,e^{im\phi}\,u(r)\big\}\,; \quad l,m \in \mathbb{Z}$$

are invariant subspaces of the operator $\widetilde{\mathcal{K}}_\varphi$, i.e., $\widetilde{\mathcal{K}}_\varphi : \mathcal{H}^{[l;m]} \mapsto \mathcal{H}^{[l;m]}$, so $\widetilde{\mathcal{K}}_\varphi = \sum_{l,m\in\mathbb{Z}} \oplus \widetilde{\mathcal{K}}_\varphi^{[l;m]}$ and, consequently,

$$\sigma(\widetilde{\mathcal{K}}_\varphi) = \overline{\bigcup_{l,m\in\mathbb{Z}} \sigma\Big(\widetilde{\mathcal{K}}_\varphi^{[l;m]}\Big)}\,.$$

The partial operators $\widetilde{\mathcal{K}}_\varphi^{[l;m]}$ *act in* $L_2[0,R]$ *as*

$$\widetilde{\mathcal{K}}_\varphi^{[l;m]} : u(r) \mapsto \int_0^R \big(u(r)\,\varphi(s)\,\Lambda_{0,0}(r,\rho) - u(s)\,\varphi(x)\,\Lambda_{l,m}(r,\rho)\big)\,d\rho\,, \tag{118}$$

where the kernels $\Lambda_{l,m}(r,\rho)$ *are*

$$\Lambda_{l,m}(r,\rho) = 4\,L \int_0^\pi d\theta \cos\theta \int_0^\pi d\phi \cos\phi \left[L\,\phi + \big(r^2 + \rho^2 - 2\,r\,\rho\,\cos\phi\big)\right]^{-1/2}. \tag{119}$$

Theorem 14 reduces the spectral problem for the operators $\widetilde{\mathcal{K}}_\varphi$ to the countable set of the spectral problem for the 1D partial operators $\widetilde{\mathcal{K}}_\varphi^{[l;m]}$.

Theorem 14. *For any acceptable biangular-symmetric field* $\varphi(\mathbf{x}) = \varphi(r)$ *having the toroidal support* $\operatorname{supp}\varphi = T_{R,Y}$*, the spectrum of the corresponding operators* $\sigma(\widetilde{\mathcal{K}}_\varphi)$ *is discrete and non-negative. Its discrete spectrum* $\sigma_d(\widetilde{\mathcal{K}}_\varphi)$ *is given by the following countable set of eigenvalues:*

$$\sigma_d(\widetilde{\mathcal{K}}_\varphi) = \big\{\nu_{n,\varphi}^{[l,m]}\big\}_{n\in\mathbb{Z}_+}^{l,m\in\mathbb{Z}}\,, \tag{120}$$

where $\nu_{n,\varphi}^{[l,m]}$ *are the eigenvalues of the partial operators* $\widetilde{\mathcal{K}}_\varphi^{[l;m]}$ *and obey the following estimates:*

$$0 \le \nu_{n,\varphi}^{[l,m]} \le \big(\varepsilon_\varphi + 2\,L\,R\,A_\varphi\big)\left[L\,R^5\mu_n + \operatorname{Si}(m\pi/2)\,8\pi^2 R A_\varphi \varepsilon_\varphi^{-1}\right]. \tag{121}$$

In particular, for the stepwise-homogeneous field $\varphi(\mathbf{x}) \equiv \chi_{T_{R,Y}}(\mathbf{x})$, Theorem 14 implies

$$0 \le \nu_{n,0}^{[l,m]} \le \left[L\,R^5\mu_n + \operatorname{Si}(m\pi/2)\right].$$

5. New class of special functions generated by the operators $\mathcal{K}_\varphi$ in higher dimensions

This section is devoted to the interesting side results manifesting deep links of the problems under consideration with other fields of mathematics. Namely, we address here the new class of special functions $\Xi_N^{[\mathbf{k}]}(z)$, generated by the kernels of the operators $\mathcal{K}_\varphi$ in higher dimensions $M = N + 1 \ge 2$ [13, 28, 30] (see Remark 8 in Sect. 4.2).

This section is organized as follows. In Sect. 5.1 we provide some general remarks on the functions $\Xi_N^{[\mathbf{k}]}$. Sections 5.2 and 5.3 are devoted to the particular cases $N = 1$ and $N = 2$, respectively. We have expressed functions $\Xi_1^{[k]}$ and $\Xi_2^{[\mathbf{k}]}$ in terms of the Gauss hypergeometric functions ${}_2F_1$ and Clausen's generalized hypergeometric functions ${}_3F_2$, respectively. We suspect that the higher rank ($N \ge 3$) functions $\Xi_N^{[\mathbf{k}]}(z)$ could be expressed in terms of (probably multivariate) hypergeometric functions. We also present the differential equations satisfied by these Ξ-functions. A study of the higher rank Ξ-functions $M \ge 4$ has a rather mathematical interest and will be performed later.

5.1. General remarks on the special functions $\Xi_N^{[\mathbf{k}]}(z)$)

We define [28]

$$\Xi_N^{[\mathbf{k}]}(z) := \int_0^{2\pi} d\theta_1 \int_0^{2\pi} d\theta_2 \cdots \int_0^{2\pi} d\theta_N \, \cos(k_l\theta_l) \left[1 + z^2 - 2\, z\, N^{-1} \sum_{l=1}^{N} \cos\theta_l\right]^{-1/2}, \tag{122}$$

where $\mathbf{k} := \{k_1, k_2, \ldots, k_N\} \in \mathbb{Z}_+^N$.

Let us note that [13] introducing function

$$\mathcal{F}_N(x,\, \Theta) := \left[1 + x^2 - 2\, x\, N^{-1} \sum_{l=1}^{N} \cos\theta_l\right]^{-1/2},$$

we have

$$\mathcal{F}_N(x,\, \Theta) = \sum_{\mathbf{k}\in\mathbf{Z}_+^N} \Xi_N^{[\mathbf{k}]}(x)\, \cos k_l\theta_l\,. \tag{123}$$

Actually, functions $\Xi_N^{[\mathbf{k}]}(x)$ are the coefficients of the decomposition of $\mathcal{F}_N(x,\, \Theta)$ in Fourier series with respect to variable $\Theta \in [0, \pi] \times \mathbf{Z}_+^N$. Below we consider the cases $N = 1$ and $N = 2$ (in Sects. 5.2 and 5.3, respectively).

5.2. Rank-1 special functions $\Xi_1^{[k]}(z)$

In this subsection we discuss the simplest case of rank-1 functions $\Xi_1^{[k]}(z)$, mostly following the results of [13, 28, 30]. These functions are defined by formula (99) with $N = 1$, where $k \in \mathbb{Z}$.

In papers [13, 28] a simplified notation $\xi_k(x) := \Xi_1^{[k]}(x)$ was used for the case $N = 1$. Here we follow [30] and keep the universal notation $\Xi_N^{[\mathbf{k}]}$ for all $N \geq 1$ to avoid inconveniences.

Representation (133) implies (taking $\theta = 0$, $\theta = \pi$ and $\theta = \pi/2$)

$$\frac{1}{1 \mp x} = \sum_{k=0}^{\infty} (\pm 1)^k\, \Xi_1^{[k]}(x)\,; \qquad \frac{1}{\sqrt{1 + x^2}} = \sum_{k=0}^{\infty} (-1)^k\, \Xi_1^{[k]}(x)\,. \tag{124}$$

For any function $G(\theta)$ decomposable as

$$G(\theta) = \sum_{k=0}^{\infty} G^{[k]}\, \cos k\,\theta\,; \quad G^{[k]} = \frac{1}{\pi} \int_0^{\pi} G(\theta)\, \cos k\,\theta\, d\theta$$

(with obvious generalization for dimensions $N \geq 2$) the following relation is valid:

$$\sum_{k=0}^{\infty} G^{[k]}\, \Xi_1^{[k]}(x) = \int_0^{\pi} \mathcal{F}_1(x,\, \theta)\, G(\theta)\, d\theta\,. \tag{125}$$

The inverse Fourier representation gives

$$\Xi_1^{[k]}(x) = \int_0^{\pi} \mathcal{F}_1(x,\, \theta) \cos k\,\theta\, d\theta \tag{126}$$

For the case $N = 1$ the formulae (122) and (136) imply

$$\frac{1}{\sqrt{1 + x^2 - 2\,x\,\cos\theta}} = \sum_{k=0}^{\infty} \Xi_1^{[k]}(x)\,\cos k\,\theta\,. \tag{127}$$

Comparing with the generating function for Legendre polynomials $P_k(z)$ [31, 34]:

$$\frac{1}{\sqrt{1 + x^2 - 2\,x\,z}} = \sum_{k=0}^{\infty} x^k\,P_k(z)$$

we get the following decomposition of functions $\Xi_1^{[k]}(x)$ into the power series:

$$\Xi_1^{[k]}(x) = \sum_{l=0}^{\infty} \tau_l^{[k]}\,x^l\,, \tag{128}$$

where

$$\tau_l^{[k]} := \frac{1}{\pi}\int_0^{\pi} P_l(\cos\theta)\,\cos k\,\theta\,d\theta\,. \tag{129}$$

Given representation [31, 34]

$$P_l(\cos\theta) = \frac{(2l-1)!!}{2^{\,l-1}\,l!}\sum_{m=0}^{\infty}\alpha_{l,m}\,\cos(l-2m)\,\theta\,,$$

$$\alpha_{l,m} := \frac{(2m-1)!!}{m!}\,\frac{l(l-1)(l-2)\cdots(l-m+1)}{(2l-1)(2l-3)(2l-5)\cdots(2l-2m+1)}\,,$$

one can calculate [13]

$$\tau_l^{[k]} = \begin{cases} 0\,, & \text{if } l+k \text{ is odd,} \\ \dfrac{(2l-1)!!}{2^l\,l!}\left(\alpha_{l,\frac{l+k}{2}} + \alpha_{l,\frac{|l-k|}{2}}\right), & \text{if } l+k \text{ is even}\,. \end{cases} \tag{130}$$

Representations (138), (139) together with the well-known relation [31, 34] for the Legendre polynomials

$$(l+1)\,P_{l+1}(z) + l\,P_{l-1}(z) = (2l+1)\,z\,P_l(z)$$

give the following formula:

$$\left[x\,\frac{d}{dx} + \frac{1}{2}\right]\left(\Xi_1^{[k]}(x) + \Xi_1^{[k+2]}\right) = \left[\left(1 + x^2\right)\frac{d}{dx} + x\right]\Xi_1^{[k+1]}(x)\,. \tag{131}$$

The corresponding calculations are straightforward but boring, and will be published elsewhere.

Choosing in Eq. (127) $\cos\theta = x/2$, we get a decomposition of unit:

$$1 \;=\; \sum_{k=0}^{\infty}\Xi_1^{[k]}(2\,\cos\theta)\,\cos k\,\theta\,; \quad \pi/3 \;<\; \theta \le \pi/2\,. \tag{132}$$

Similarly, choosing $\cos\theta = (2x)^{-1}$, we get

$$2\,\cos\theta = \sum_{k=0}^{\infty}\Xi_1^{[k]}\Big(\frac{1}{2\,\cos\theta}\Big)\,\cos k\,\theta\;; \quad 0 \le \theta < \pi/3\,. \tag{133}$$

For $\theta = 0$, this implies another decomposition of unit:

$$1 = \frac{1}{2}\sum_{k=0}^{\infty}\Xi_1^{[k]}(1/2)\,. \tag{134}$$

Note that [28]

$$\Xi_1^{[0]}(x) = \frac{1}{1+x}\mathbf{K} \tag{135}$$

and

$$\Xi_1^{[1]}(x) = \frac{1}{1+x}\mathbf{K}\left(\frac{2\sqrt{x}}{1+x}\right) - \frac{1+x}{2x}\left.\frac{d\mathbf{E}(t)}{dt}\right|_{t=\frac{2\sqrt{x}}{1+x}}, \tag{136}$$

where $\mathbf{K}(x)$ and $\mathbf{E}(x)$ stand for the complete elliptic integrals of the first and second kind [34], respectively.

Writing P_n for the nth Legendre polynomial [31, 18.7.9], we have the following generating function ([31, 18.12.11], [33, (2.5.42)]:

$$\frac{1}{\sqrt{1+x^2-2xz}} = \sum_{n=0}^{\infty} P_n(z)x^n. \tag{137}$$

Substituting then leads to

$$\Xi_1^{[k]}(x) = \sum_{n=0}^{\infty}\tau_n^{[k]}x^n$$

with

$$\tau_n^{[k]} = \frac{1}{\pi}\int_0^{\pi} P_n(\cos(\theta))\cos(k\theta)d\theta.$$

(see [28] for details). On the other hand, according to $\lambda = 1/2$ case of [31, 18.5.11],

$$P_n(\cos(\theta)) = \sum_{j=0}^{n}\frac{(1/2)_j(1/2)_{n-j}}{j!(n-j)!}\cos((n-2j)\theta)\,,$$

where $(a)_k = \Gamma(a+k)/\Gamma(a)$ is the rising factorial. Hence, we have

$$\begin{aligned}\tau_n^{[k]} &= \frac{1}{\pi}\int_0^{\pi} P_n(\cos(\theta))\cos(k\theta)d\theta \\ &= \frac{1}{\pi}\sum_{j=0}^{n}\frac{(1/2)_j(1/2)_{n-j}}{j!(n-j)!}\int_0^{\pi}\cos((n-2j)\theta)\cos(k\theta)d\theta.\end{aligned}$$

In view of [31, 4.26.10-11]

$$\int_0^{\pi}\cos((n-2j)\theta)\cos(k\theta)d\theta = \begin{cases}0, & n-2j\neq k,\\ \pi/2, & n-2j=k\neq 0,\\ \pi, & n-2j=k=0.\end{cases} \tag{138}$$

After elementary calculation this amounts to

$$\tau_n^{[k]} = \frac{1}{2}\frac{(1/2)_{(n-k)/2}(1/2)_{(n+k)/2}}{((n-k)/)!((n+k)/2)!},$$

where $n \geq k$ and $n-k$ is even. If $n-k$ is odd $\tau_n^{[k]} = 0$. Hence, changing $n-k$ to $2m$ we get:

$$\begin{aligned}\Xi_1^{[k]}(x) &= \frac{1}{2}\sum_{n=k}^{\infty}\frac{(1/2)_{(n-k)/2}(1/2)_{(n+k)/2}}{((n-k)/2)!((n+k)/2)!}x^n \\ &= \frac{1}{2}\sum_{m=0}^{\infty}\frac{(1/2)_m(1/2)_{m+k}}{m!(m+k)!}x^{2m+k} \\ &= \frac{(1/2)_k x^k}{2k!}\sum_{m=0}^{\infty}\frac{(1/2)_m(1/2+k)_m}{(1+k)_m m!}x^{2m} \\ &= \frac{(1/2)_k x^k}{2k!}\,{}_2F_1(1/2, 1/2+k; k+1; x^2),\end{aligned} \tag{139}$$

where ${}_2F_1$ is the Gauss hypergeometric function whose main properties can be found, e.g., in [31, Chap. 15] or [32, Chap. 8]. In the second equality we have used the easily verifiable identity $(a)_{m+k} = (a)_k(a+k)_m$ was used.

One can obtain the recurrent relation for the functions $\Xi_1^{[k]}$ [28]. The result is

Theorem 15. *The functions $\Xi_1^{[k]}(x)$ obey the functional relation*

$$\left[x\,\frac{d}{dx} + \frac{1}{2}\right]\left(\Xi_1^{[k]}(x) + \Xi_1^{[k+2]}(x)\right) = \left[\left(1+x^2\right)\frac{d}{dx} + x\right]\Xi_1^{[k+1]}(x)\,. \tag{140}$$

The functional relations (140) allow for another direct expression of the functions $\Xi_1^{[k+1]}(x)$ through $\Xi_1^{[k]}(x)$ and $\Xi_1^{[k+2]}(x)$. Namely [28]

Corollary 5. *The functions $\Xi_1^{[k]}(x)$ obey the functional relation*

$$\begin{aligned}\Xi_1^{[k+1]}(x) = \frac{\Xi_1^{[k]}(x) + \Xi_1^{[k+2]}(x)}{1+x^2} &- \frac{1}{2\sqrt{1+x^2}} \\ &- \int_{-1}^{1}\frac{1-x'^2}{(1+x'^2)^{3/2}}\left[\Xi_1^{[k]}(x') + \Xi_1^{[k+2]}(x')\right]dx'\,.\end{aligned} \tag{141}$$

The following simple result [30] is valid.

Lemma 4. *If a function $G(z)$ obeys the second order differential equation*

$$Q_2(z)D^2G(z) + Q_1(z)DG(z) + Q_0(z)G(z) = 0, \tag{142}$$

where $D = \frac{d}{dz}$ and $Q_m(z)$ are functional parameters, then the function

$$H(z) := Cz^{\alpha}G(z)\,,\ C = \text{Const},$$

obeys the second order differential equation

$$P_2(z)D^2H(z) + P_1(z)DH(z) + P_0(z)H(z) = 0, \tag{143}$$

with

$$P_2(z) \equiv Q_2(z)\,, \quad P_1(z) \equiv Q_1(z) - 2\alpha z^{-1} Q_2(z),$$
$$P_0(z) \equiv Q_0(z) - \alpha z^{-1} Q_1(z) + \alpha(\alpha+1) z^{-2} Q_2(z).$$

Proof. The claim follows from substituting $G(z) = C^{-1} z^{-\alpha} H(z)$ into Eq. (142), trivial calculations and multiplication of the result by z^α [30]. □

Representation (139) expresses the functions $\Xi_1^{[k]}(x)$ in terms of the Gauss hypergeometric function ${}_2F_1$, which determines its analytic and asymptotic (in the neighborhood of $x = 1$ in particular) properties. We take $z = x^2$. The function ${}_2F_1$ from (139) satisfies the hypergeometric differential equation (see [32, 8.23], [31, 15.10.1], [39, 2.1(1)] or [33, (2.1.6)])

$$\Big[z(1-z)D^2 + \big(k+1-(k+2)z\big)D - \big(1/4 + k/2\big)\Big]\,{}_2F_1\,(1/2, 1/2+k; k+1; z) = 0\,.$$

Now we use Lemma 4 with $G(z) \equiv \Xi_1^{[k]}(\sqrt{z})$, $C = (1/2)_k/(2k!)$, $Q_2(z) \equiv z(1-z)$, $Q_1(z) \equiv k+1-(k+2)z$, $Q_0 \equiv 1/4 + k/2$, $\alpha = k/2$. As $z = x^2$, $D = \frac{d}{dz} = \frac{1}{2x}\frac{d}{dx}$ and $D^2 = (4x^2)^{-1}\frac{d^2}{dx^2} - (4x^3)^{-1}\frac{d}{dx}$. This gives the following result [30]:

Theorem 16. *Functions* $\Xi_1^{[k]}(x)$ *obey the second-order differential equation*

$$\left[x^2(1-x^2)\frac{d^2}{dx^2} + x(1-3x)\frac{d}{dx} + x^2(k^2-1) - k^2\right]\Xi_1^{[k]}(x) = 0. \tag{144}$$

To continue the functions $\Xi_1^{[k]}(x)$ to the complex plane $x \to z \in \mathbb{C}$ one can use the representation (139) expressing these functions in terms of the Gauss hypergeometric function ${}_2F_1$.

Following Fuchs' terminology [33, Sect. 1.1], the point x of equation (144) is called *singular* if the functional coefficient at d^2/dx^2 vanishes at this point, and (in our case) point $x = \infty$. Hence, for the functions $\Xi_1^{[k]}(z)$ there are three such points: $z = 0$, $z = 1$ and $z = \infty$. According to [33, Chap. 2], all these singular points are regular.

5.3. Rank-2 special functions $\Xi_2^{[\mathbf{k}]}(z)$

In this subsection we discuss the functions $\Xi_2^{[\mathbf{k}]}(z)$, mostly following the results of [30]. These functions are defined by formula (99) with $N = 2$, where $\mathbf{k} = (k_1, k_2) \in \mathbb{Z}^2$. The main result is the following theorem [30].

Theorem 17. *Suppose* $0 \le k_1 \le k_2$ *are integers,* $\mathbf{k} = (k_1, k_2)$*. Put* $s = \lfloor (k_2 - k_1)/2 \rfloor$*. Then for* $x \in \mathbb{R}$

$$\begin{aligned}\Xi_2^{[\mathbf{k}]}(x) = {} & \frac{\pi^2 (1/2)_{k_1+k_2} (2x)^{k_1+k_2}}{4^{k_1+k_2+1} k_1! k_2!} \\ & \cdot \sum_{j=0}^{s} \frac{((k_1-k_2)/2)_j ((k_1-k_2+1)/2)_j (k_1+k_2+1/2)_{2j} x^{2j}}{(k_1+1)_j (k_2+1)_j (k_1+k_2+1)_j j!} \\ & \cdot {}_3F_2\left(\begin{matrix} 1/2+j, k_1+1/2+j, k_1+k_2+1/2+2j \\ k_2+1+j, k_1+k_2+1+j \end{matrix} \,\middle|\, -x^2 \right), \end{aligned} \tag{145}$$

where ${}_3F_2$ *denotes Clausen's generalized hypergeometric function* [31, Chap. 16]*. Note that* $(0)_0 = 1$ *in the above formula.*

Corollary 6. *Under the assumption of Theorem* 17 *suppose in addition that* $k_2 - k_1 \le 1$*. Then*

$$\Xi_2^{[\mathbf{k}]}(x) = \frac{\pi^2 (1/2)_{k_1+k_2} (2x)^{k_1+k_2}}{4^{k_1+k_2+1} k_1! k_2!} {}_3F_2\left(\begin{matrix} 1/2, k_1+1/2, k_1+k_2+1/2 \\ k_2+1, k_1+k_2+1 \end{matrix} \,\middle|\, -x^2 \right). \tag{146}$$

The proof of Theorem 17 is rather technical and is based on the following key lemma.

Lemma 5. *For given non-negative integers* l, k_1, k_2 *define*

$$A_l(k_1, k_2) := \iint\limits_{0 \le \theta_1, \theta_2 \le \pi} (\cos(\theta_1) + \cos(\theta_2))^l \cos(k_1\theta_1) \cos(k_2\theta_2) d\theta_1 d\theta_2. \tag{147}$$

Then

$$A_l(k_1, k_2) = \begin{cases} 0, & l \not\equiv k_1 + k_2 \pmod 2 \text{ or } l < k_1 + k_2, \\ \frac{\pi^2}{2^l} \binom{k_1+k_2}{k_1} \dfrac{(k_1+k_2+1)_{2N}^2}{(k_1+1)_N (k_2+1)_N (k_1+k_2+1)_N N!}, & \\ \qquad l \equiv k_1 + k_2 \pmod 2 \text{ and } l \ge k_1 + k_2, & \end{cases} \tag{148}$$

where $N = (l - k_1 - k_2)/2$.

Lemma 5 was proved in [30] through an application of Zeiberger's algorithm [38, section 3.11] (using, for instance, Fast Zeilberger Package by Peter Paule and Markus Schorn [41]).

To continue the functions $\Xi_2^{[k]}(x)$ to the complex plane $x \to z \in \mathbb{C}$ one can use the representation (145) expressing these functions in terms of the Clausen's generalized hypergeometric function ${}_3F_2$. Note, that contrary to the case $N = 1$, where the singular points of the function $\Xi_1^{[k]}(z)$ are real ($z = \pm 1$, for $N = 2$ the singular points of the function $\Xi_2^{[\mathbf{k}]}(z)$ are $z = \pm i$.

The following result, similar to Theorem 16, is valid [30]:

Theorem 18. *For* $\mathbf{k} = (k_1, k_2)$ *such that* $k_2 - k_1 \le 1$, *functions* $\Xi_2^{[k]}(x)$ *obey the third-order differential equation*

$$\Big[x^3(1-x^2)\frac{d^3}{dx^3} + x^2\Big((k_1-k_2+6)(x^2-1)+9\Big)\frac{d^2}{dx^2} - x\Big((k_1+k_2)^2(x^2+1) + (k_2-k_1-7/3)(3x^2-1) - 10/3\Big)\frac{d}{dx} + x^2\Big((k_1+k_2)^2 - 1) + (k_1-k_2)(k_1+k_2)^2\Big]\Xi_2^{[\mathbf{k}]}(x) = 0\,. \tag{149}$$

Proof. The proof provided in [30] follows from the straightforward calculation and is based on the equation [40]

$$\big[\mathcal{T}(\mathcal{T}+b_1-1)(\mathcal{T}+b_2-1) - z(\mathcal{T}+a_1)(\mathcal{T}+a_2)(\mathcal{T}+a_3)\big]{}_3F_2\left(\begin{matrix}a_1, a_2, a_3\\ b_1, b_2\end{matrix}\,\middle|\, z\right) = 0\,,$$

where the operator $\mathcal{T}$ is defined by

$$\mathcal{T} := z\frac{d}{dz}\,.$$

Let us note, that for the "lowest mode", i.e., in case $k_1 = k_2 = 0$, Theorem 18 implies

$$\Big[x^3(1-x^2)\frac{d^3}{dx^3} + x^2\Big(6(x^2-1)+9\Big)\frac{d^2}{dx^2} + \frac{x}{3}\Big(7(3x^2-1)+10\Big)\frac{d}{dx} + x^2\Big]\Xi_2^{[\mathbf{0}]}(x) = 0\,. \qquad \square$$

6. Links to other fields of mathematics

In this section we consider links of operators under investigation with some other fields of mathematics (infinite Jacobi matrices with unbounded entries, maximinimal principle and spectral estimations, inverse problems).

6.1. Infinite Jacobi matrices with unbounded entries

In 1D case one can decompose solutions of the spectral problem $K_\varphi u = \lambda u$ through Legendre polynomials

$$u(x) = \sum_{k=0}^{N} u_k p_k(x) \tag{150}$$

and rewrite the spectral problem in l_k, so that

$$u_k \equiv \mathcal{B}_{kn} = \sum_{m=0}^{k} u_n^k; \quad u_n^k = \sum_{k=0}^{n} \mu_k - \int_{-1}^{1} \frac{p_k(s)p_n(s)}{|x-s|}\, ds\,. \tag{151}$$

Let us consider the simplest case $\varphi(x) = \alpha_0 p_0(x) + \alpha_1 p_1(x)$. In this case

$$\mathcal{B}_{kk} = \alpha_0 \mu_k\,;\ \mathcal{B}_{k\pm 1k} = \alpha_1 \int_{-1}^{1}\int_{-1}^{1} \frac{p_k(s)p_n(s)}{|x-s|}\, dsdx\,, \tag{152}$$

so diag $\mu_k - \{\mathcal{B}_{kn}\}$ is a 3-diagonal Jacobi matrix with unbounded entries.

6.2. Maximinimal principle and spectral estimation

As shown above, under the conditions of Theorem 4 the operator K_φ is semibounded from below, has purely discrete spectrum, and is selfadjoint in the Hilbert space $L_2([-1,1], dx/\varphi(x))$. Due to the maximinimal principle [1, 2], the nth eigenvalue of the operator K_φ can be calculated as follows:

$$\tau_n^\varphi = \max_{\Phi_n \subset \mathcal{D}_\varphi} \inf_{u \in \Phi_n, \mathbf{I}u\mathbf{I}_\varphi = 1} \langle K_\varphi u, u \rangle_\varphi \,, \tag{153}$$

where $\dim \Phi_n = n$. The operator K_0 is also semibounded from below, has purely discrete spectrum, and is selfadjoint in the Hilbert space $L_2[-1,1]$. Thus, due to the maximinimal principle its eigenvalues $\mu_n = 2\sum_{j=0}^{n} j^{-1}$ are

$$\mu_n = \max_{\Phi_n \subset \mathcal{D}_0} \inf_{u \in \Phi_n, \mathbf{I}u\mathbf{I}_\varphi = 1} (K_0 u, u) \,. \tag{154}$$

Under the conditions of Theorem 4, the domains $\mathcal{D}_\varphi$ and $\mathcal{D}_0$ of the operators K_0 and K_φ, respectively, coincide: $\mathcal{D}_\varphi = \mathcal{D}_0$. This allows us to get the following estimate for for the eigenvalues of the operator K_φ (see [10], Sect. 3.5):

$$\mu_n \min_{x \in [-1,1]} \varphi(x) - \max_{x \in [-1,1]} |(K_0 \varphi)(x)| \le \tau_n \le \mu_n \max_{x \in [-1,1]} \varphi(x) + \max_{x \in [-1,1]} |(K_0 \varphi)(x)|. \tag{155}$$

Due to the conditions (5), (6), the following estimate can be specified:

$$\varepsilon_\varphi \mu_n - 2A_\varphi \le \tau_n^\varphi \le (\varepsilon_\varphi + 2A_\varphi)\mu_n + 2A_\varphi \,. \tag{156}$$

7. Inverse problems (reconstruction of the external field $\varphi(x)$ through the spectrum of the operator $\mathcal{K}_\varphi$) in 1D case

In Sect. 4 above we considered the inverse problems on graphs. However, this problem an be generalized for any admissible domains in $\mathbb{R}$. Namely, the function $f(x)$ is expressed through the Riesz potential [76], so one an use the following formula:

$$\mathcal{I}_\alpha = f * T_\alpha = \frac{1}{c_\alpha} \int_{\mathbb{R}} \frac{f(s)}{|x-s|^{N-\alpha}} \, ds \,, \tag{157}$$

where $c_\alpha \equiv \pi^{1/2} 2^\alpha \frac{\Gamma(\alpha/2)}{\Gamma(N-\alpha)/2)}$.

Taking $\alpha = N-1$, one gets

$$\mathcal{I}_{N-1} = \frac{1}{c_{N-1}} \int_{\mathbb{R}} \frac{f(s)}{|x-s|} \, ds \,. \tag{158}$$

In the same manner one can reconstruct the external field $\varphi(x)$ through the spectrum of the operator $\mathcal{K}_\varphi$. Indeed, given function $q_\varphi(x)$ from formula (158) one gets

$$\varphi(x) = \int_{\mathbb{R}} \frac{q_\varphi(s)}{|x-s|} \, ds \,. \tag{159}$$

As an example, let us consider the simplest case when

$$q_\varphi(x) = q^{ac}(x) + \sum_n \gamma_n \delta(x - \lambda_n),$$

where $q^{ac}(x)$ is an absolutely-continuous function and singularities at $x = \lambda_n$ are responsible for the discrete spectrum of the operator $\mathcal{K}_\varphi$ located in the points $x = \lambda_n$. As an example,we consider $\varphi(x) = e^{-\beta x}$. Using formula (159), we get the representation

$$\varphi(x) = \frac{1-x}{\beta}\, e^{-\beta x} + \sum_n \frac{\gamma_n}{x - \lambda_n}.$$

The operators K_φ in quasi-1D structures, i.e., graphs, were considered in [29]. Quantum graphs have been the subject of numerous investigations addressing various aspects [50]–[72]. Mostly Schrödinger operators in the graphs have been studied. There graphs were used as quasi-1D structures to investigate the dynamics of the corresponding matter relaxation processes defined by the operator K_φ given by the representation (5) with the domain Ω being a (compact) graph G. In [29] the operators K_φ were considered in the graphs G of specific type. A set of consequent simplifications was introduced and the overview of the corresponding spectral results was provided. Below we formulate the inverse problem for integral-difference operators.

Let us formulate the inverse problem for integral-difference operators underlying the matter relaxation processes in general. In quantum scattering this problem reads as the reconstruction of the potential given the scattering data [73]. For integral-difference operators $\mathcal{K}_\varphi$ the inverse problem is to reconstruct the field φ given the physically measurable data from the corresponding matter relaxation processes.

Namely, let $\mathcal{U}(\mathbf{x}, t)$ be the matter density in the spatial point $\mathbf{x} \in \mathbb{R}^N$ at the time moment $t \geq 0$. We formulate the inverse problem as follows.

Definition 5. *The inverse problem for the operator $\mathcal{K}_\varphi$ is to find the field $\varphi(\mathbf{x})$, $\mathbf{x} \in \Omega \subset \mathbb{R}^N$ given the matter density $\mathcal{U}(\mathbf{x}, 0)$ and $\mathcal{U}(\mathbf{x}, t_0)$ at some time $t_0 > 0$.*

Actually, the problem goes to the inversion of the Riesz potential operator (see, e.g., [74]). Namely, in formula (7.21) of [74] one can take $\alpha = N - 1$ and thus invert the operator

$$f(\mathbf{x}) := J_\varphi(\mathbf{x}) = \int_{\mathbb{R}^N} \frac{\varphi(\mathbf{s})}{|\mathbf{x} - \mathbf{s}|} d^N\mathbf{s} \tag{160}$$

as

$$\begin{aligned} \varphi(\mathbf{x}) &= J_\varphi^{-1}(\mathbf{x}) \\ &= \frac{\Gamma(1/2)}{2^{N-1}\pi^{N/2}\Gamma((N-1)/2)} \\ &\quad \cdot \lim_{\epsilon \to 0} \int_{\mathbb{R}^N} \left[\frac{1}{(|\mathbf{y}|^2 + \epsilon^2)^{N-1/2}} - \frac{N+1}{N-1} \frac{\epsilon}{(|\mathbf{y}|^2 + \epsilon^2)^{N+1/2}} \right] f(\mathbf{x} - \mathbf{y})\, d^N\mathbf{y}\,. \end{aligned} \tag{161}$$

The latter formula is sufficient for any $N \geq 2$, as due to Eq. (66) the inversion of the operator K_φ looks like

$$\varphi(\mathbf{x}) = \frac{1}{u(\mathbf{x})} J_\varphi^{-1} \left[1 - \int_{\mathbb{R}^N} \frac{u(\mathbf{x})}{|\mathbf{x}-\mathbf{s}|} \frac{1}{u(\mathbf{x})} d^N\mathbf{s} \right]^{-1} J_\varphi^{-1} K_\varphi u \,. \tag{162}$$

Therefore, if we know the distribution of the matter density $\mathcal{U}(\mathbf{x}, t_0)$ at the time moment $t_0 \geq 0$, we can take $u(\mathbf{x}) = \mathcal{U}(\mathbf{x}, t_0) = \exp\{-t_0\}\mathcal{U}(\mathbf{x}, 0)$ and apply the previous formula.

Usually the inverse problems are considered for Schrödinger operators [50]–[75]. Here we turn to the inverse problems for operator $\mathcal{K}_\varphi$, i.e., to the reconstruction of the external field $\varphi(\mathbf{x})$ through some observable data, and apply it to simple graphs [50]–[72]. In our previous paper we [29] we have considered compact graphs G with finite number a of the brunches. Without loss of generality, using a simple change of variables such graphs can be represented as

$$G = \bigcup_{l=1}^{a} [-1, 1], \quad l = 1, 2, 3, \ldots, a, \; a \geq 1 \,. \tag{163}$$

The operators K_φ in the graph G are defined as

$$K_{\widehat{\varphi}}^{\widehat{g}} = \sum_{k=1}^{a} \sum_{l=1}^{a} \oplus K_{\varphi_l}^{[kl]} \,, \tag{164}$$

where $\widehat{\varphi} := \{\varphi_l(x_l)\}_{l=1}^a$ and $\widehat{g} := \{g_{kl}\}_{k,l=1}^a$. Without loss of generality we can assume that for all $l = 1, 2, \ldots, a$ the copies of the interval $[-1, 1] \ni x_l$ intersect in one common point $x_1 = x_2 = x_3 = x_l = \cdots = x_a = 0$. In this point matter flows from lth interval $[-1, 1] \ni x_l$ to kth interval $[-1, 1] \ni x_k$ and vice versa can take place.

The trivial case $a = 2$ is just the situation of interval $x \in [-1, 1]$. As shown in [6, 10], in this case the operator K_φ can be represented as

$$K_\varphi = \varphi \circ K_0 - (K_0\varphi) \,, \tag{165}$$

where φ and $(K_0\varphi)$ stand for the operators of the multiplication by the corresponding functions. The operator K_0 is exactly solvable [6, 10]. Its eigenvalues are

$$\mu_0 = 0, \quad \mu_n = \sum_{j=1}^{n} j^{-1} \,, \; n \geq 1 \,,$$

and the corresponding eigenfunctions are Legendre polynomials $p_n(x)$. Representation (165) allows for the following approach.

The transition intensity is determined by the matrix elements of $a \times a$ matrix $\widehat{g}$, such that $g_{kl} > 0$ if $k \neq l$ and $g_{ll} = 0 \, \forall l = 1, 2, 3, \ldots, a$. This generates additional matter incoming and outgoing processes. Namely, if $a \geq 2$ for any $l = 1, 2, 3, \ldots, a$

these leads to the additional term $B^{[l]}$ in the operator $K_{\varphi_l}^{[kl]}$ given by

$$B^{[l]} : u_l(x_l) \mapsto \sum_{k=1}^{a} g_{kl} \, \frac{u_l(x_l)\,\varphi_l(0) - u_l(0)\,\varphi_l(x_l)}{|x_l|} \,, \tag{166}$$

which leads to the representation

$$K_{\varphi_l}^{[kl]} = K_{\varphi_l} + B^{[l]} \,. \tag{167}$$

For the domain under consideration $u_l(x_l) \in C^1[-1,1]$ and acceptable functions $\varphi_l(x_l) \in C^1[-1,1]$ every term in the right-hand side of the representation (16) is obviously finite. Note, that if $a = 1$, i.e., the graph $G = [-1,1]$ is trivial, the term $B^{[1]}$ disappears and one just gets the original operator $K_{\varphi_l}^{[11]} = K_{\varphi_1}$ introduced and considered in [6]–[10].

There are several possible steps to simplify the operators $B^{[l]}$ given by representation (16). Namely,

(S1) All functions $\varphi_l(x_l)$ are assumed to be identical, i.e., $\varphi_l(x_l) \equiv \varphi(x_l)$ $\forall l = 1,2,3,\dots,a$. Then for the operators $B^{[l]}$ we have

$$B^{[l]} : u_l(x_l) \mapsto \sum_{k=1}^{a} g_{kl} \, \frac{u_l(x_l)\,\varphi(0) - u_l(0)\,\varphi(x_l)}{|x_l|} \,. \tag{168}$$

(S2) All transition coefficients are similar, i.e., $g_{kl} = g > 0$ $\forall l \neq k$, $l,k = l = 1,2,3,\dots,a$, and $g_{ll} = 0$ $\forall l = 1,2,3,\dots,a$. Then, assuming simultaneously (S1) and (S2), we get

$$B^{[l]} : u_l(x_l) \mapsto \; g\,a \, \frac{u_l(x_l)\,\varphi(0) - u_l(0)\,\varphi(x_l)}{|x_l|} \,. \tag{169}$$

(S3) Functional parameter $\varphi(s) \equiv 1$ is trivial.

Assuming simultaneously (S1)–(S3), one gets

$$B^{[l]} : u_l(x_l) \mapsto \; g\,a \, \frac{u_l(x_l) - u_l(0)}{|x_l|} \,. \tag{170}$$

Therefore, under the simplifying assumptions (S1)–(S3), the operator $K_{\varphi_l}^{[kl]}$ turns into

$$K_0^{[kl]} : u(x) \;\mapsto (K_0 u)(x) + g\,a \, \frac{u(x) - u(0)}{|x|} \,, \tag{171}$$

where $(K_0 u)(x) = \int_{-1}^{1} \frac{u(x)-u(s)}{|x-s|} ds$.

Under the simplifying assumptions (S1)–(S3), let us consider the spectral problem for the operator $K_0^{[kl]}$

$$\big(K_0^{[kl]} f\big)(x) = \lambda f(x) \,. \tag{172}$$

Representing $f(x)$ through the normalized Legendre polynomials $p_n(x)$

$$f(x) = \sum_{n \geq 0} f_n \, p_n(x) \,, \tag{173}$$

by straightforward calculation, one gets

$$\mu_m f_m + g\,a \sum_{n\geq 0} \gamma_{mn} f_n = \lambda f_m \,, \tag{174}$$

where

$$\gamma_{mn} := \int_{-1}^{1} \frac{p_n(s) - p_n(0)}{|s|}\, p_m(s)\, ds \,. \tag{175}$$

Using integral inequalities [42], we have

$$0 \leq |\gamma_{mn}|^2 \leq \int_{-1}^{1} \left| \frac{p_n(s) - p_n(0)}{s} \right|^2 ds = 2 \left| \frac{d}{dx}\, p_n(x) \right|^2_{x=0} . \tag{176}$$

As (see, e.g., [45])

$$\left| \frac{d}{ds}\, p_n(s) \right|^2_{s=0} = \frac{1}{\sqrt{2}} \,, \tag{177}$$

we have $-1 \leq \gamma_{mn} \leq 1$.

Therefore, every eigenvalue μ_m of the operator K_0 (see Theorem 1) generates the interval $[\mu_m - 1, \mu_m + 1]$ where the eigenvalues λ_ν of the operator $K_0^{[kl]}$ can be located, i.e., for any $m \geq 0$ there can exist the eigenvalue

$$\sigma_d\big(K_0^{[kl]}\big) \ni \lambda_\nu \in [-ga, ga] \bigcup_{m=2}^{\infty} \left[2ga \sum_{j=2}^{m} \frac{1}{j} \,,\, 2ga + 2ga \sum_{j=2}^{m} \frac{1}{j} \right] . \tag{178}$$

The eigenfunctions $f_\nu(x)$ corresponding to the eigenvalues λ_ν are given by the Legendre functions of the first and the second kind [45],

$$f_\nu(x) = \omega_\nu\, P_\nu(x) + \widetilde{\omega}_\nu\, Q_\nu(x) \tag{179}$$

with arbitrary constants ω_ν and $\widetilde{\omega}_\nu$;

$$P_\nu(x) \equiv F\Big(-\nu, \nu+1; 1; \frac{1-x}{2}\Big) \,; \tag{180}$$

$$Q_\nu(x) \equiv \frac{\Gamma(\nu+1)\,\Gamma(1/2)}{2\nu+1\,\Gamma(3/2)}\, x^{-\nu-1}\, F\left(\frac{\nu+2}{2}, \frac{\nu+1}{2}; \frac{\nu+3}{2}; \frac{1}{x^2} \right) , \tag{181}$$

where

$$F\big(\varkappa_1, \varkappa_2; \varkappa_3; \xi\big) = 1 + \frac{\varkappa_1 \cdot \varkappa_2}{\varkappa_3 \cdot 1}\, \xi + \frac{\varkappa_1 \cdot (\varkappa_1+1) \cdot \varkappa_2 \cdot (\varkappa_2+1)}{\varkappa_3 \cdot (\varkappa_3+1) \cdot 1 \cdot 2}\, \xi^2 + \frac{\varkappa_1 \cdot (\varkappa_1+1) \cdot (\varkappa_1+2) \cdot \varkappa_2 \cdot (\varkappa_2+1) \cdot (\varkappa_2+2}{\varkappa_3 \cdot (\varkappa_3+1) \cdot (\varkappa_3+2) \cdot 1 \cdot 2 \cdot 3}\, \xi^3 + \cdots$$

stands for the Gauss hypergeometric function [45].

The above discussion can be formulated as

Theorem 19. *Under the simplifying conditions* (S1)–(S3) *every eigenvalue μ_m of the operator K_0 generates the interval $[\mu_m - 1, \mu_m + 1]$ where the eigenvalues λ_ν of the operator $K_0^{[kl]}$ can be located, i.e., for any $m \geq 0$ there can exist the eigenvalue*

$$\lambda_\nu \in [\mu_m - 1, \mu_m + 1] \,. \tag{182}$$

The corresponding eigenfunctions $f_\nu(x)$ *are given by formula* (179).

8. Conclusions and further tasks

The present paper provides the mathematical results obtained since 1997 in the spectral analysis of integral-difference operators defined by formula (1), and outlines their so far known physical applications. Additionally, links with various fields of mathematics have been traced and some side results there (e.g., in the theory of special functions) have been obtained.

However, there are still remain encouraging open problems (listed below), determining the possible directions of further studies in the field. Namely,

PR 1. The spectral analysis of the operators $\mathcal{K}_\varphi$ has been reasonably developed only for the acceptable (in the sense of Definition 1) functional parameters $\varphi(\mathbf{x})$, even in the 1D case $M = 1$. The most strong and not always physically natural demand in Definition 1 is due to the condition (6), requesting the homogeneous separation of the function $\varphi(\mathbf{x})$ from zero in its support $\operatorname{supp}\varphi = \Omega \subset \mathbb{R}^M$. That means that for some physically important cases like the Gaussian distributions (see Sect. 3.5) the developed technique is not applicable. The reason is that it is essentially based on the resolvent comparison approach for the operators $\mathcal{K}_\varphi$ and the reference operator $\mathcal{K}_0$ (corresponding to the step-constant function $\varphi(\mathbf{x}) \equiv 1$ for $\mathbf{x} \in \Omega$ and $\varphi(\mathbf{x}) \equiv 0$ for $\mathbf{x} \in \mathbb{R}^M \backslash \Omega$). The reason is that if the condition (6) is violated, the restricted to $L_2(\Omega)$ operator of the multiplication by the function $1/\varphi(\mathbf{x})$ is not always bounded, so the resolvent comparison approach fails. Moreover, although in some other cases this operator of the multiplication is still bounded (e.g., for $1/\varphi(\mathbf{x}) \in L_2(\Omega)$, due to Hölder inequality [42]), as the operators $\mathcal{K}_\varphi$ are considered in the domains $\mathcal{D}_\varphi \ni u(\mathbf{x})$ such that $u(\mathbf{x})|_\Omega \subset L_2(\Omega)$, important estimates for $\min_{\mathbf{x}\in\Omega} \varphi(\mathbf{x})$ do not exist. Thus, study of the operators $\mathcal{K}_\varphi$ beyond the condition (6) is an open problem.

PR 2. Currently we know only one exactly solvable operator in the family $\mathcal{K}_\varphi$. That is the reference operator $\mathcal{K}_0$ i the 1D case, corresponding to the step-constant function $\varphi(x) \equiv 1$ for $x \in \Omega = (a, b) \subset \mathbb{R}$ and $\varphi(\mathbf{x}) \equiv 1$ and $\varphi(\mathbf{x}) \equiv 0$ for $x \in \mathbb{R}\backslash[a, b]$). The eigenvalues μ_n, the absolutely continuous spectrum $\sigma_{ac}(\mathcal{K}_0) = \mathbb{R}_+$ and the corresponding (generalized) eigenfunctions $u_n(x)$ $(n = 0, 1, 2, \dots)$ and $u_\lambda(x)$ $(\lambda \in \mathbb{R}_+\backslash\{\mu_n\})$ are known exactly (see Sect. 3.2) are known precisely. However, such results are so far not known for any other function $\varphi(x)$ in the 1D case and for any function $\varphi(\mathbf{x})$ in higher dimensions $M \geq 2$.

PR 3. In the 1D case, for the restricted reference operator K_0 it is shown (see Sect. 3.2) that K_0 commutes with the differential operator $\mathcal{L}$ generating the Legendre polynomials. For any other functions φ in all dimensions $M \geq 1$ such differential or pseudo-differential operators commuting with K_φ are not known.

PR 4. In higher dimensions $M \geq 2$ the obtained results are valid for the admissible domains Ω, i.e., for countable sets of finite intervals with finite total volume in the 1D case $M = 1$ (see Definition 2) and for compact convex domains $\Omega \subset \mathbb{R}^M$ in higher dimensions $M \geq 2$ (see Definition 2). Moreover, the sound results for $M \geq 2$ are so far obtained if Ω is a completely admissible domain (the pseudo-torus $\Omega = \widehat{\mathbf{T}}^{M-1}$), see Definition 3). A generalization for the domains $\Omega \subset \mathbb{R}^M$ would be interesting.

PR 5. Spectral estimations through the quadratic form approach in higher dimensions $M \geq 2$ (see Sect. 4.2) so far have been obtained for the functional parameters $\varphi(\mathbf{x})$ having specific symmetry in the specific domains Ω. That are a disk or a ring in $\mathbb{R}^2$ (see Sect. 4.3) and a torus or a cylinder in $\mathbb{R}^3$ (see Sect. 4.4). The corresponding results for other types of the functions $\varphi(\mathbf{x})$ and other domains are not known yet .

PR 6. The properties of the special functions $\Xi_N^{[\mathbf{k}]}$ have been investigated only for the rank-1 ($N = 1$) and the rank-2 ($N = 2$) functions (see Sects. 5.2 and 5.3, respectively). The properties of the higher rank $N \geq 3$ special functions $\Xi_N^{[\mathbf{k}]}$ have not been studied yet. One may suspect that they can be expressed in terms of the higher Clausen's generalized hypergeometric functions ${}_pF_q$, but that should be the subject of further investigations.

PR 7. The recurrent relation for $\Xi_2^{[\mathbf{k}]}$ (like (140) or (141) for $\Xi_1^{[\mathbf{k}]}$, with more terms) have not been obtained yet.

PR 8. For other domains the operators $\mathcal{K}_\varphi$ generate special functions differ from the functions $\Xi_N^{[\mathbf{k}]}$, which study may become an interesting problem. As shown in [77], the integral-difference operators $K_{\varphi_l}^{[kl]}$ in the physical space being the graph G defined in (14) has similar to the original operator K_φ spectral properties. The set of the consequent simplifications (S1)–(S3) allows for the detailed spectral estimations for the operators. Above we have considered the specific graphs G, which are the finite sets of the intervals $[-1, 1]$ intersecting in the common point $x_1, x_2, x_3, \dots, x_a = 0$, $l = 1, 2, 3, \dots, a < \infty$.

However, the situation an be generalized for other types of graphs G. Namely, one can consider graphs G with richer structure and turn to the following tasks:

PR 9. Graph G is a finite set of intervals $[-1, 1]$ intersecting in various points.

PR 10. Graph G contains a subset of semi-bounded intervals $[0, \infty)$.

PR 11. Graph G contains the infinite number of bounded and/or semi-bounded intervals intersecting in various points.

PR 12. Graph G contains a finite or countable set of the loops.

PR 13. Condition of the compactness of the field $\varphi(x)$ support Ω is not prescribed.

PR 14. Ω is not a quasi-1D structure (graph), but is a 2D or 3D domain.

All these situations can also be simplified in the manner similar to that used for the considered graphs G and described at (S1)–(S3).

Other encouraging tasks are related to the inverse problems for the operators K_φ. In the simplest case they can be formulated as follows:

PR 15. To restore the field $\varphi(\mathbf{x})$, $\mathbf{x} \in \Omega \subset \mathbb{R}^N$, given the geometric form of the domain Ω and the spectral decomposition of the operator K_φ.

PR 16. To restore the field $\varphi(\mathbf{x})$, $\mathbf{x} \in G$ the transition coefficients matrix $\widehat{g}$, given the geometric form of the graph G and the spectral decomposition of the operator K_φ in G.

Another key task is

PR 17. To single out the physical meaning of the graphs G of various types, i.e., to trace more specific relations between the scattering in quantum graphs and the considered integral-difference operators in these graphs.

Currently, we stay with all these encouraging problems.

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Inverse problem for integral-difference operators on graphs

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Abstract. We consider the inverse problem for integral-difference operators underlying the dynamics of the matter relaxation in external attractive fields for quasi-1-dim structures (graphs). Under specific simplifying conditions the solution of this inverse problem is obtained. The further possible generalization for a broader set of graphs and other domains is discussed and the corresponding encouraging investigations are proposed.

Keywords. Quantum graphs, integral-difference operators, inverse problem.

1. Introduction and background

Integral-difference operators in non-equilibrium statistical physics models [1, 2] appeared in 1990s [3]. Originally they described the collision processes in 1D systems. Their spectral properties describe the rates of the system to go to the equilibrium (Lyapunov exponentials). At the same years a rigorous mathematical approach for the spectral analysis for such operators was proposed [4]–[8]. Later on another physical interpretation of such operators (matter relaxation in external attractive fields) was introduced both in 1D and for higher dimensions N [9]–[12]. For higher dimensions $N = 2, 3$, it was based in the specific interest of physicists [14]–[24]. The quadratic form approach has been used for the appropriate spectral estimations both in 1D and in higher dimensions $N = 2, 3$ [9]. The general review was recently published [12]. The corresponding operators for simple graphs were studied in [13].

Generally, the operators under the consideration look like

$$\mathcal{K}_\varphi : u(\mathbf{x}) \mapsto \int_{\mathbb{R}^N} \frac{u(\mathbf{x})\,\varphi(\mathbf{s}) - u(\mathbf{s})\,\varphi(\mathbf{x})}{|\mathbf{x}-\mathbf{s}|}\, d^N\mathbf{s} \tag{1}$$

where function $\varphi(\mathbf{x})$ is a functional parameter called as external field. Usually, the so-called *acceptable* functions $\varphi(\mathbf{x})$ [9, 12] are used, i.e., such that satisfy the following conditions:

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Definition 1. *Function* $\varphi(\mathbf{x})$ *in* $\mathbb{R}^N$ *is called as acceptable function if it is non-negative, summable, of Lipshitz-1 class and is uniformly separated from zero in its support* $\operatorname{supp}\varphi = \Omega \subset \mathbb{R}^N$ [8, 9, 12]. *Namely, this means that* $\varphi(\mathbf{x})$ *satisfies the following conditions:*

$$0 \le \varphi(\mathbf{x}) \in L_1(\mathbb{R}^N)\,; \tag{2}$$

$$\exists\, A_\varphi \ge 0 :\ |\varphi(\mathbf{x}) - \varphi(\mathbf{s})| \le A_\varphi\, |\mathbf{x}-\mathbf{s}|, \quad \forall \mathbf{x},\mathbf{s} \in \Omega\,; \tag{3}$$

$$\exists\, \varepsilon_\varphi > 0 :\ \varphi(\mathbf{x}) \ge \varepsilon_\varphi, \quad \forall\, \mathbf{x} \in \Omega\,. \tag{4}$$

Note that the conditions (2) and (4) can be satisfied simultaneously only if the domain $\operatorname{supp}\varphi(\mathbf{x}) := \Omega \subset \mathbb{R}^N$ has a finite volume $\mathrm{Vol}(\Omega) < \infty$.

Operators $\mathcal{K}_\varphi$ are defined [12] as the operators given by (1) in

$$L_2(\mathbb{R}^N) \cap L_1(\mathbb{R}^N) \cap C^1(\mathbb{R}^N).$$

The physical meaning of the operators $\mathcal{K}_\varphi$ and the domain $\operatorname{supp}\varphi = \Omega \subset \mathbb{R}^N$ is discussed in [12]. The technique introduced in [4] and used in [5]–[12] makes it important to consider the so-called *restricted* operators

$$K_\varphi : u(\mathbf{x}) \,\mapsto \int_\Omega \frac{u(\mathbf{x})\,\varphi(\mathbf{s}) - u(\mathbf{s})\,\varphi(\mathbf{x})}{|\mathbf{x}-\mathbf{s}|}\, d^N\mathbf{s}, \quad \mathbf{x} \in \Omega\,. \tag{5}$$

Actually, the operators K_φ determine the matter relaxation processes in external fields $\varphi(\mathbf{x})$ [9, 12].

Let us note that 1D case $N = 1$ brings a specific difficulty. Indeed, for any $N \ge 2$ the integrands in the representations (5) can be considered separately, as they are summable, i.e.,

$$K_\varphi : u(\mathbf{x}) \,\mapsto u(\mathbf{x}) \int_\Omega \frac{\varphi(\mathbf{s})}{|\mathbf{x}-\mathbf{s}|}\, d^N\mathbf{s} - \varphi(\mathbf{x}) \int_\Omega \frac{u(\mathbf{s})}{|\mathbf{x}-\mathbf{s}|}\, d^N\mathbf{s}\,. \tag{6}$$

Contrary, in 1D case $N = 1$ the representation (6) is not valid and one has to deal with the representation

$$K_\varphi : u(x) \,\mapsto \int_{-1}^{1} \frac{u(x)\,\varphi(s) - u(s)\,\varphi(x)}{|x-s|}\, d^N s\,, \tag{7}$$

which is not an integral operator.

The exact results even in 1D case [4, 8, 12] were so far obtained only for the so-called reference operator K_0, which is corresponding to the trivial functional parameter $\varphi(x) \equiv 1$ for $x \in \Omega = [-1, 1]$ and $\varphi(x) \equiv 0$ outside of the interval $[-1, 1]$ [4, 8, 12].

The operators K_φ in quasi-1D structures, i.e., graphs, were considered in [13]. Quantum graphs have been the subject of numerous investigations addressing various aspects [28]–[54]. Mostly Schrödinger operators in the graphs have been studied. There graphs were used as quasi-1D structures to investigate the dynamics of the corresponding matter relaxation processes defined by the operator K_φ given by the representation (5) with the domain Ω being a (compact) graph G. In [13] the operators K_φ were considered in the graphs G of specific type. A set of consequent simplifications was introduced and the overview of the corresponding spectral results was provided. In Sect. 2 we formulate the inverse problem for integral-difference operators. Section 3 is devoted to this inverse problem in simple graphs. In Sect. 4 we discuss further tasks.

2. Formulation of the inverse problem for integral-difference operators

Let us formulate the inverse problem for integral-difference operators underlying the matter relaxation processes in general. In quantum scattering this problem reads as the reconstruction of the potential given the scattering data [55]. For integral-difference operators $\mathcal{K}_\varphi$ the inverse problem is to reconstruct the field φ given the physically measurable data from the corresponding matter relaxation processes.

Namely, let $\mathcal{U}(\mathbf{x},t)$ be the matter density in the spatial point $\mathbf{x}\in\mathbb{R}^N$ at the time moment $t\geq 0$. We formulate the inverse problem as follows.

Definition 2. *The inverse problem for the operator $\mathcal{K}_\varphi$ is to find the field $\varphi(\mathbf{x})$, $\mathbf{x}\in\Omega\subset\mathbb{R}^N$ given the matter density $\mathcal{U}(\mathbf{x},0)$ and $\mathcal{U}(\mathbf{x},t_0)$ at some time $t_0>0$.*

Actually, the problem goes to the inversion of the Riesz potential operator (see, e.g., [56]). Namely, in formula (7.21) of [56] one can take $\alpha = N-1$ and thus invert the operator

$$f(\mathbf{x}) := J_\varphi(\mathbf{x}) = \int_{\mathbb{R}^N} \frac{\varphi(\mathbf{s})}{|\mathbf{x}-\mathbf{s}|}\,d^N\mathbf{s} \tag{8}$$

as

$$\begin{aligned}\varphi(\mathbf{x}) &= J_\varphi^{-1}(\mathbf{x})\\ &= \frac{\Gamma(1/2)}{2^{N-1}\pi^{N/2}\Gamma((N-1)/2)}\\ &\quad\cdot \lim_{\epsilon\to 0}\int_{\mathbb{R}^N}\left[\frac{1}{(|\mathbf{y}|^2+\epsilon^2)^{N-1/2}} - \frac{N+1}{N-1}\frac{\epsilon}{(|\mathbf{y}|^2+\epsilon^2)^{N+1/2}}\right] f(\mathbf{x}-\mathbf{y})\,d^N\mathbf{y}\,.\end{aligned} \tag{9}$$

The latter formula is sufficient for any $N\geq 2$, as due to Eq. (6) the inversion of the operator K_φ looks like

$$\varphi(\mathbf{x}) = \frac{1}{u(\mathbf{x})}\,J_\varphi^{-1}\left[1-\int_{\mathbb{R}^N}\frac{u(\mathbf{x})}{|\mathbf{x}-\mathbf{s}|}\,\frac{1}{u(\mathbf{x})}d^N\mathbf{s}\right]^{-1} J_\varphi^{-1}\;K_\varphi u\,. \tag{10}$$

Therefore, if we know the distribution of the matter density $\mathcal{U}(\mathbf{x},t_0)$ at the time moment $t_0\geq 0$, we can take $u(\mathbf{x}) = \mathcal{U}(\mathbf{x},t_0) = \exp\{-t_0\}\mathcal{U}(\mathbf{x},0)$ and apply the previous formula.

In 1D and quasi-1D cases (graphs) the situation is different. As mentioned above, the representation (6) is not valid in these cases, therefore one has to use the representation (7). This problem is considered below in Sect. 3.

3. The inverse problem for integral-difference operators in simple graphs

In our previous paper we [13] we have considered compact graphs G with finite number a of the branches. Without loss of generality, using a simple change of variables [13] such graphs can be represented as

$$G = \bigcup_{l=1}^{a} [-1,1], \quad l = 1,2,3,\ldots,a;\ a \ge 1\,. \tag{11}$$

The operators K_φ in the graph G are defined as

$$K_{\widehat{\varphi}}^{\widehat{g}} = \sum_{k=1}^{a}\sum_{l=1}^{a} \oplus K_{\varphi_l}^{[kl]}\,, \tag{12}$$

where $\widehat{\varphi} := \{\varphi_l(x_l)\}_{l=1}^a$ and $\widehat{g} := \{g_{kl}\}_{k,l=1}^a$. Without loss of generality, we can assume that for all $l = 1,2,\ldots,a$ the copies of the interval $[-1,1] \ni x_l$ intersect in one common point $x_1 = x_2 = x_3 = x_l = \cdots = x_a = 0$. In this point matter flows from the lth interval $[-1,1] \ni x_l$ to the kth interval $[-1,1] \ni x_k$ and vice versa can take place.

The trivial case $a = 2$ is just the situation of interval $x \in [-1,1]$. As shown in [4, 8, 12], in this case the operator K_φ can be represented as

$$K_\varphi = \varphi \circ K_0 - (K_0\varphi)\,, \tag{13}$$

where φ and $(K_0\varphi)$ stand for the operators of the multiplication by the corresponding functions. The operator K_0 is exactly solvable [4, 8, 12]. Its eigenvalues are

$$\mu_0 = 0, \quad \mu_n = \sum_{j=1}^{n} j^{-1}, \quad n \ge 1\,,$$

and the corresponding eigenfunctions are Legendre polynomials $p_n(x)$. Representation (13) allows for the following approach.

The transition intensity is determined by the matrix elements of $a \times a$ matrix $\widehat{g}$, such that $g_{kl} > 0$ if $k \ne l$ and $g_{ll} = 0\ \forall l = 1,2,3,\ldots,a$. This generates additional matter incoming and outgoing processes. Namely, if $a \ge 2$ for any $l = 1,2,3,\ldots,a$ these leads to the additional term $B^{[l]}$ in the operator $K_{\varphi_l}^{[kl]}$ given by

$$B^{[l]} : u_l(x_l) \mapsto \sum_{k=1}^{a} g_{kl}\, \frac{u_l(x_l)\,\varphi_l(0) - u_l(0)\,\varphi_l(x_l)}{|x_l|}\,, \tag{14}$$

which leads to the representation

$$K_{\varphi_l}^{[kl]} = K_{\varphi_l} + B^{[l]}\,. \tag{15}$$

For the domain under consideration $u_l(x_l) \in C^1[-1,1]$ and acceptable functions $\varphi_l(x_l) \in C^1[-1,1]$ every term in the right-hand side of the representation

(16) is obviously finite. Note, that if $a = 1$, i.e., the graph $G = [-1, 1]$ is trivial, the term $B^{[1]}$ disappears and one just gets the original operator $K_{\varphi_l}^{[11]} = K_{\varphi_1}$ introduced and considered in [4]–[12].

There are several possible steps to simplify the operators $B^{[l]}$ given by representation (16). Namely,

(S1) All functions $\varphi_l(x_l)$ are assumed to be identical, i.e., $\varphi_l(x_l) \equiv \varphi(x_l)$ $\forall l = 1, 2, 3, \ldots, a$. Then for the operators $B^{[l]}$ we have

$$B^{[l]} : u_l(x_l) \mapsto \sum_{k=1}^{a} g_{kl} \, \frac{u_l(x_l)\, \varphi(0) - u_l(0)\, \varphi(x_l)}{|x_l|} \,. \tag{16}$$

(S2) All transition coefficients are similar, i.e., $g_{kl} = g > 0$ $\forall l \neq k$, $l, k = l = 1, 2, 3, \ldots, a$, and $g_{ll} = 0$ $\forall l = 1, 2, 3, \ldots, a$. Then, assuming simultaneously (S1) and (S2), we get

$$B^{[l]} : u_l(x_l) \mapsto \; g\, a \, \frac{u_l(x_l)\, \varphi(0) - u_l(0)\, \varphi(x_l)}{|x_l|} \,. \tag{17}$$

(S3) Functional parameter $\varphi(s) \equiv 1$ is trivial.

Assuming simultaneously (S1)–(S3), one gets

$$B^{[l]} : u_l(x_l) \mapsto \; g\, a \, \frac{u_l(x_l) - u_l(0)}{|x_l|} \,. \tag{18}$$

Therefore, under the simplifying assumptions (S1)–(S3), the operator $K_{\varphi_l}^{[kl]}$ turns into

$$K_0^{[kl]} : u(x) \; \mapsto (K_0 u)(x) + g\, a \, \frac{u(x) - u(0)}{|x|} \,, \tag{19}$$

where $(K_0 u)(x) = \int_{-1}^{1} \frac{u(x) - u(s)}{|x-s|} ds$.

Under the simplifying assumptions (S1)–(S3), let us consider the spectral problem for the operator $K_0^{[kl]}$

$$\big(K_0^{[kl]} f\big)(x) = \lambda f(x) \,. \tag{20}$$

Representing $f(x)$ through the normalized Legendre polynomials $p_n(x)$

$$f(x) = \sum_{n \geq 0} f_n \, p_n(x) \,, \tag{21}$$

by straightforward calculation one gets

$$\mu_m \, f_m + g\, a \sum_{n \geq 0} \gamma_{mn} \, f_n = \lambda f_m \,, \tag{22}$$

where

$$\gamma_{mn} := \int_{-1}^{1} \frac{p_n(s) - p_n(0)}{|s|} \, p_m(s) \, ds \,. \tag{23}$$

Using integral inequalities [57], we have

$$0 \le |\gamma_{mn}|^2 \le \int_{-1}^{1} \left| \frac{p_n(s) - p_n(0)}{s} \right|^2 ds = 2 \left| \frac{d}{dx}\, p_n(x) \right|^2_{x=0} . \tag{24}$$

As (see, e.g., [27])

$$\left| \frac{d}{ds}\, p_n(s) \right|^2_{s=0} = \frac{1}{\sqrt{2}} , \tag{25}$$

we have $-1 \le \gamma_{mn} \le 1$.

Therefore, every eigenvalue μ_m of the operator K_0 (see Theorem 1) generates the interval $[\mu_m - 1, \mu_m + 1]$ where the eigenvalues λ_ν of the operator $K_0^{[kl]}$ can be located, i.e., for any $m \ge 0$ there can exist the eigenvalue

$$\sigma_d\big(K_0^{[kl]}\big) \ni \lambda_\nu \in [-ga, ga] \bigcup_{m=2}^{\infty} \left[2ga \sum_{j=2}^{m} \frac{1}{j} \, , \, 2ga + 2ga \sum_{j=2}^{m} \frac{1}{j} \right] . \tag{26}$$

The eigenfunctions $f_\nu(x)$ corresponding to the eigenvalues λ_ν are given by the Legendre functions of the first and the second kind [27],

$$f_\nu(x) = \omega_\nu \, P_\nu(x) + \tilde{\omega}_\nu \, Q_\nu(x) \tag{27}$$

with arbitrary constants ω_ν and $\tilde{\omega}_\nu$ as well as

$$P_\nu(x) \equiv F\Big(-\nu, \nu + 1; 1; \frac{1-x}{2}\Big) ; \tag{28}$$

$$Q_\nu(x) \equiv \frac{\Gamma(\nu+1)\,\Gamma(1/2)}{2\nu + 1\,\Gamma(3/2)}\, x^{-\nu-1}\, F\left(\frac{\nu+2}{2}, \frac{\nu+1}{2}; \frac{\nu+3}{2}; \frac{1}{x^2} \right) , \tag{29}$$

where

$$F\big(\varkappa_1, \varkappa_2; \varkappa_3; \xi\big) = 1 + \frac{\varkappa_1 \cdot \varkappa_2}{\varkappa_3 \cdot 1}\, \xi + \frac{\varkappa_1 \cdot (\varkappa_1 + 1) \cdot \varkappa_2 \cdot (\varkappa_2 + 1)}{\varkappa_3 \cdot (\varkappa_3 + 1) \cdot 1 \cdot 2}\, \xi^2 + \frac{\varkappa_1 \cdot (\varkappa_1 + 1) \cdot (\varkappa_1 + 2) \cdot \varkappa_2 \cdot (\varkappa_2 + 1) \cdot (\varkappa_2 + 2}{\varkappa_3 \cdot (\varkappa_3 + 1) \cdot (\varkappa_3 + 2) \cdot 1 \cdot 2 \cdot 3}\, \xi^3 + \cdots$$

stands for the Gauss hypergeometric function [27].

The above discussion can be formulated as

Theorem 1. *Under the simplifying conditions* (S1)–(S3)*, every eigenvalue μ_m of the operator K_0 generates the interval $[\mu_m - 1, \mu_m + 1]$ where the eigenvalues λ_ν of the operator $K_0^{[kl]}$ can be located, i.e., for any $m \ge 0$ there can exist the eigenvalue*

$$\lambda_\nu \in [\mu_m - 1, \mu_m + 1] . \tag{30}$$

The corresponding eigenfunctions $f_\nu(x)$ are given by formula (27)*.*

4. Conclusion and further tasks

As shown above in [13], the integral-difference operators $K^{[kl]}_{\varphi_l}$ in the physical space being the graph G defined in (14) has similar to the original operator K_φ spectral properties. The set of the consequent simplifications (S1)–(S3) allows for the detailed spectral estimations for the operators . Above we have considered the specific graphs G, which are the finite sets of the intervals $[-1, 1]$ intersecting in the common point $x_1, x_2, x_3, \ldots, x_a = 0$, $l = 1, 2, 3, \ldots, a < \infty$.

However, the situation an be generalized for other types of graphs G. Namely, one can consider graphs G with more reach structure and turn to the following tasks:

(T1) Graph G is a finite set of intervals $[-1, 1]$ intersecting in various points.
(T2) Graph G contains a subset of semi-bounded intervals $[0, \infty)$.
(T3) Graph G contains the infinite number of bounded and/or semi-bounded intervals intersecting in various points.
(T4) Graph G contains a finite or countable set of the loops.
(T5) Condition of the compactness of the field $\varphi(x)$ support Ω is not prescribed.
(T6) Ω is not a quasi 1D structure (graph), but is a 2D or 3D domain.

All these situations can also be simplified in the manner similar to that used for the considered graphs G and described by (S1)–(S3).

Other encouraging tasks are related to the inverse problems for the operators K_φ. In the simplest case they can be formulated as follows:

(T7) To restore the field $\varphi(\mathbf{x})$, $\mathbf{x} \in \Omega \subset \mathbb{R}^N$, given the geometric form of the domain Ω and the spectral decomposition of the operator K_φ.
(T8) To restore the field $\varphi(\mathbf{x})$, $\mathbf{x} \in G$ the transition coefficients matrix $\widehat{g}$, given the geometric form of the graph G and the spectral decomposition of the operator K_φ in G.

Another key task is

(T9) To single out the physical meaning of the graphs G of various types, i.e. to trace more specific relations between the scattering in quantum graphs [28]–[54] and the considered integral-difference operators in these graphs.

Tasks (T1)–(T9) are the subject of further investigations.

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Breeding of the running spin-waves with standing spin-modes in a quantum well

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Abstract. Spin-depending scattering is studied on a two-dimensional quantum network constructed of a quantum well with three semi-infinite quantum wires (an input wire and two terminals) attached to it. The spin-orbital interaction causing selective scattering in the network is described by the Rashba Hamiltonian. The transmission of electrons across the well from the input quantum wire to terminals is caused by the excitation of a resonance oscillatory spin-mode in the well. For thin quantum networks we suggest also an approximate formula which defines the resonance transmission of electrons across the quantum well, depending on the shape of the standing spin-mode in the quantum well.

1. Introduction

During last decade the world-community of nano-electronics is engaged in a search of new physical principles, materials and technologies on which the quantum spin-transistor may be manufactured [1, 2, 4, 3, 5, 6, 7, 8, 9, 10]. This anticipated device could become a base of the toolbox which can permit to verify the efficiency of quantum computations and test the constructions of various quantum networks.

The basic principle of the spin-transistor was suggested by the authors of [1]. The leading idea of their proposal is the use of the spin-orbital interaction [11] for creation of the spin-polarized current in the transistor channel. Actually, to produce a real device based on the mentioned principle, one should solve at least two basic problems:

1. The problem of selection of proper material with maximal spin-orbital interaction, which may permit to achieve in a 2D system a considerable spin-orbital splitting, at least for “nitrogen temperatures”; ideally, for room temperatures.
2. The problem of the introduction and withdrawal of electrons with certain value of spin polarization.

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We assume that the spin-orbital interaction is defined by the phenomenological Rashba Hamiltonian (2.2) with the parameter α, which defines numerically the features of the corresponding interaction

$$E^{\pm} = \frac{\hbar^2 k^2}{2m} \pm \alpha k, \tag{1.1}$$

and is connected directly with the spin-orbital splitting $\Delta_R = E^+ - E^-$. Generally for Kane-type materials not just the simplest formula (1.1), but another formula is true:

$$E = \sqrt{(s_i \hbar k)^2 + (m_i S_i^2)^2 \pm (2m_i S_i^2)^2 \alpha_i k} - m_i S_i^2. \tag{1.2}$$

This formula contains the saturated splitting $\Delta_R^{\max} \approx 2m_i S_i^2$, and the number i of the quantum band. Extended comparative analysis of the formulae (1.1), (1.2) may be found in [14].

According to [12, 13, 14] both the theory and an experiment vote in favor of materials $Cd_x Hg_{1-x} Te$ ($0 \le x \le 1$), where Δ_R circa 40–60 meV, and the magnitude of effective Rashba parameter is about (0.2–0.3)10^{-10} eV m. This is approximately 10 times bigger, than the parameter α in other hetero-structures studied before : $\Delta_R \approx (0.02 : 5)$ meV and $\alpha \approx (10^{-12} - 10^{-11})$ eV m. We guess that such materials as Cd, Hg, Te are most prospective for the high-temperature spintronics. Analysis done in [14, 15, 16] shows that large values of spin-orbital splitting is achieved for InAs and HgTe. All these semiconductors are representatives of the class of narrow-gap materials with the widest bands.

In semiconductors with a nearly parabolic dispersion curve $E \approx \frac{\hbar^2 p^2}{2m*}$ the magnitude of the expected splitting is at least 2 or 3 orders less than in narrow-gap materials listed above. Nevertheless in actual paper we suggest a theoretical analysis of scattering in a material with parabolic dispersion curve and the Rashba Hamiltonian just included additively, because of the universal character of the quadratic dispersion for small α. Our aim is revealing the effects of the shape of the resonance standing spin-waves in Scattering processes on the quantum well in presence of the spin-orbital interaction. Thus we make a step toward the solution of the second of above problems – the problem of introducing and withdrawal of spin-polarized electrons, – actually the problem of registration of the spin-polarization. This problem, though very popular now, still is far from the solution. Our analysis permits to connect directly the transmission coefficients across the quantum well with the shape of the resonance eigenfunctions in the well, which can be computed, for various geometry of the well, based on a standard software. This allows to approach the solution of the second problem mentioned above: the withdrawal of the spin-polarized electron current.

We develop analysis of the resonance transmission in spin-dependent scattering based on our previous papers [19, 20, 21, 26], where different variants of design of the Resonance Quantum Switch were proposed and analyzed. Similarly to the construction in [26], we observe in this paper the selective transmission of electrons across the quantum well, due to excitation of the resonance standing waves inside the well. In [26] we used the shape of the resonance eigenfunction to optimize the switching effect. In actual paper we derive the explicit basic formulae for the scattering matrix based on intermediate Hamiltonian. We construct the intermediate Hamiltonian, for given Fermi level, such that the discrete spectrum of it lies above the Fermi level. This allows to avoid perturbations on the continuous spectrum. In particular the resonances of the full Hamiltonian are connected, in case of thin networks, with the eigenvalues of the intermediate Hamiltonian by an algebraic equation. This allows to estimate the transmission coefficients across the well based on spectral data of *discrete spectrum of the intermediate Schrödinger operator* which can be obtained via straightforward computing.

An essential difference of the actual problem from [26] is the fact, that the resonance eigenfunctions in actual problem are *complex* two-component spinors. Hence we are unable optimize the filtering, as in [26], via appropriate localization of lines of zeros of the resonance mode in the well. We will optimize the selectivity of the filter depending on the shape of the well in a forthcoming paper, based on our formula for approximate transmission coefficients, in terms of the shape of the eigenfunctions of the intermediate operator in the well, for different shapes of the well.

The structure of the paper is the following. In the following section we introduce Schrödinger equations which serve the base of our analysis. In the next Sect. 3 we derive the boundary conditions for the Schrödinger equation with with spin-orbital interaction defined by the Rashba Hamiltonian (2.2). In Sect. 4 we calculate the Scattering matrix based on the Dirichlet-to-Neumann map of an intermediate Hamiltonian. Neglecting the non-resonance terms in the Dirichlet-to-Neumann map we present the transmission of an electron across the well via an excitation of the resonance oscillatory mode inside the well. Based on that we calculate in Sect. 5 the scattering matrix and reveal the resonance character of the transmission. In appendix basic properties of the intermediate hamiltonian are discussed.

Our calculations in the paper are based on the simple formula (1.1) for the spin-orbital splitting, which is valid for materials with the parabolic dispersion curve, but we pay a special attention to the role of the shape of the resonance eigenfunction in the transmission process. In the forthcoming paper we will extend our analysis of the shape-resonance transmission across the well to the most prospective narrow-gap materials for which an analog of the formula (1.2) can be derived.

2. Geometry of the filter: preliminaries

Consider a network $\Omega = \Omega_{\rm int} \cup \Omega_1 \cup \Omega_2 \cup \Omega_3$ on the plane (x, z), combined of a quantum well $\Omega_{\rm int}$ and three straight semi-infinite quantum wires $\Omega_s,\ s = 1, 2, 3$ of constant width δ attached to the well $\Omega_{\rm int}$. The one-body Hamiltonian of an electron on Ω is defined by the Schrödinger differential expressions (2.3) and (2.4), see below, with Dirichlet boundary conditions $\partial\Omega$ and appropriate boundary conditions on the common boundary Γ of the well and the wires.

Introducing the coordinate x_m along the wire, we may also assume, without restriction of generality, that the normal bottom cross-section $\gamma_m^{\rm out}$: $x_m = 0$ is selected strictly inside the wire Ω_m, just cutting the wire into two parts: the semi-infinite part ω_m situated "above" the section $\gamma_m^{\rm out}$, $x_m > 0$, and the small trapezial cut-off – the link – $\Omega_m \backslash \omega_m := \Omega_m^\varepsilon$"below" the section. Hereafter we call Ω_m *the extended wire*, to distinguish it from ω_m. We include the links Ω_m^ε, $\cup_m \Omega_m^\varepsilon := \Omega^\varepsilon$, into the extended quantum well $\Omega_{\rm int}^\varepsilon = \Omega_{\rm int} \cup \Omega^\varepsilon$, but assume that the potential of the Schrödinger equation on the links is constant and coincides with V_m, and shrinks as prescribed in Sect. 5 below. Thus the wire $\omega_m : 0 < x_m < \infty$ is attached to $\Omega_{\rm int}$ through the corresponding orthogonal cross-section $\gamma_m^{\rm out}$: $x_m = 0$, which therefore is a part of the boundary of $\Omega_{\rm int}^\varepsilon$. The common boundary $\cup_m \gamma_m^{\rm out}$ of $\Omega_{\rm out} := \cup_m \omega_m$ and $\Omega_{\rm int}^\varepsilon$ is denoted by $\Gamma^{\rm out}$. We distinguish the outer $\Gamma_+^{\rm out}$ and the inner $\Gamma_-^{\rm out}$ sides of $\Gamma^{\rm out}$. The extended quantum well $\Omega_{\rm int}^\varepsilon$ also has a piecewise smooth boundary and satisfies the bilateral cone condition but it is not assumed to be simply-connected (e.g., Fig. 1 shows a detail of a multiply-connected domain). In particular, one can imagine $\Omega_{\rm int}$ being a network of quantum wells connected by wires of finite lengths.

The quantum network considered in this paper is a partial case of a "fattened graphs" described for instance in [25], see Fig. 1. In Sects. 4 and 5 we consider the shrinking of the network. In fact we consider shrinking of the wires only. To avoid technical difficulties, we assume that the wires of the shrinking network are attached to $\Omega_{\rm int}$ on flat pieces of its boundary $\gamma_m^{\rm int}$, $\cup_m \gamma_m^{\rm int} = \Gamma^{\rm int} \subset \partial\Omega_{\rm int}$. We distinguish the outer and the inner sides $\Gamma_\pm^{\rm int}$ of $\Gamma^{\rm int}$, with respect to $\Omega_{\rm int}$. Each link Ω_m^ε is a trapezoid of height δ, with two sides $y = 0, \delta$ parallel to the sides of the wire ω_m, and the middle line $y = \delta/2$. The hight of the trapezoid coincides with the width δ of the wire. The shape the link is defined by two additional parameters, the minimal angle $\pi/2 - \theta$ at the bottom and the length $\delta\varepsilon$ of the center line. Then the upper and bottom sides of the trapezoid are equal to $\delta[\varepsilon \mp 2^{-1}\tan\theta]$.

We assume that the parameters of the links fulfill some geometrical condition which is used in shrinking process. In simplest case, when the tensor of effective mass is isotropic and constant, this condition means that the link is relatively small, and the angle θ is small enough, so that the wires are attached to the quantum well "almost orthogonally", this condition says:

$$\varepsilon^2 < 6^{-1}. \tag{2.1}$$

In course of shrinking each semi-infinite wire and each link shrinks self-similarly, $\delta = \delta_1 \times \delta$ and ε, δ_1 are constant, see Sect. 5. We supply details of the shrinking network with the label δ, for instance, the links Ω_m^ε of the shrinking networks are denoted by Ω_m^δ, to emphasis the dependence of them from δ. Similarly, the wires are denoted by ω_m^δ, and the extended quantum well is denoted by $\Omega_{\rm int}^\delta$. Note that the extended quantum well $\Omega_{\rm int}^\delta$ contains the shrinking links, hence the shape of it is also changing in the course of shrinking.

The potential on the wires is constant, and on the well it is defined by the horizontal component of the macroscopic electric field $\mathcal{E}$ parallel to the plane of the device: $V(x,z) = \mathcal{E}e\,(x\nu_x + z\nu_z) + V_0$, with $\nu \parallel (x,z)$-plane. The normal component of the electric field $\mathcal{E} = |\mathcal{E}|e_y$ is large on the quantum well, but is absent in the extended wires. This field does not contribute to the potential on the well, but is responsible for the spin-orbital interaction described by the Rashba Hamiltonian, see below (2.2). The wave-function Ψ of the electron is presented by the spinor $(\psi_1,\ \psi_2)$, and the spin-orbital interaction is taken in form of Rashba Hamiltonian [11]: as a cross-product of the vector σ of Pauli matrices $\sigma = (\sigma_x,\, \sigma_y,\, \sigma_z)$ and the vector p of momentum of the electron:

$$H_R = \alpha\,[\sigma,\ p]\,, \tag{2.2}$$

here α is proper scalar factor defined by the properties of the material and by the magnitude of the normal component of the electric field $\mathcal{E}$. The one-body Hamiltonian $L_{\rm int}$ of electron on the well, with Dirichlet boundary condition is defined by the Schrödinger operator, with appropriate boundary conditions, see the next section:

$$\frac{\hbar^2}{2m_0} Lu = -\frac{\hbar^2}{2m*}\,\triangle\, u + V(x,z)u + \alpha[\sigma_z\ p_x - \sigma_x\ p_z]u, \tag{2.3}$$

where $\alpha[\sigma_z\ p_x - \sigma_x\ p_z] = (H_R)_y$ is the y-component (2.2). The Rashba Hamiltonian is not self-adjoint in the space $L_2(\Omega)$ but being added to the 2D Schrödinger operator, produces a self-adjoint operator in $L_2(\Omega_{\rm int})$. We assume that the Schrödinger equation on the wires ω_s contains an anisotropic tensor of effective mass:

$$\frac{\hbar^2}{2m_0} l u_{\rm out} = -\frac{\hbar^2}{2m^{\parallel}}\,\frac{d^2 u_{\rm out}}{dx^2} - \frac{\hbar^2}{2m^{\perp}}\,\frac{d^2 u_{\rm out}}{dy^2}, \quad 0 < y < \delta,\, 0 < x < \infty, \tag{2.4}$$

and the width of the wires is constant and equal to δ. We neglect the spin-orbital interaction in the wires. Imposing appropriate matching boundary conditions on the sum $\Gamma^{\rm out} = \sum_{s=1}^{3} \gamma_s^{\rm out}$ of the bottom sections of the wires ω_m, and Dirichlet boundary conditions on $\partial\Omega$, we define the Hamiltonian $\frac{\hbar^2}{2m_0}\mathcal{L}$ of an electron on the network. The corresponding operator $\frac{\hbar^2}{2m_0}\mathcal{L}^*$ without any boundary conditions on $\Gamma^{\rm int}$ is not symmetric and has a non-trivial boundary form, see next section. Hereafter we distinguish the outer and the inner sides of the boundary, in particular the outer and the inner sides $\Gamma_{\pm}^{\rm int,out}$ of $\Gamma^{\rm int,out}$.

Considering shrinking networks we impose special assumptions onto the potential in the wires such that the Fermi level remains, in course of shrinking, in the middle of the conductivity band, see Sect. 5 below.

Following [26] we consider the scattering problem on the network Ω and calculate the transmission coefficients from the input wire ω_1 to the terminals $\omega_2,\ \omega_3$ across the well. These coefficients depend on the spin and energy of electrons, on the shape of the well, and on the positions of the contacts $\gamma_{2,3}$ on the boundary $\partial\Omega_{\rm int}$ and may be manipulated via the change of the direction and magnitude of the horizontal component of the electric field. In Sect. 4 we calculate the scattering matrix, which defines the transmission coefficients. The corresponding conductance for electrons with different spins may be obtained from our results based on Landauer–Buttiker formulae, see [17, 18].

3. Boundary conditions

It is convenient to assume that the boundary data of the spinors u on the inner and outer side of the boundary $\partial\Omega_{\rm int}$ are defined as:

$$u_{-,{\rm int}}(x) = \lim_{\varepsilon\to 0} u(x-\varepsilon n_x) = u(x),\ \ x\in\partial\Omega_{\rm int},\ \ u_{+,{\rm int}}\big|_{\gamma_m^{\rm int}} = u_m,\ u_{\rm out}\big|_{\partial\Omega_{\rm int}\setminus\Gamma} = 0.$$

Then we are able to introduce the jumps and the mean values of the spinors on the common boundary $\Gamma^{\rm int}$ of the quantum well $\Omega_{\rm int}$ and the extended quantum wires $\Omega_{\rm out} = \cup_m\Omega_m$, by the following expressions:

$$\begin{aligned}
[u]\big|_{\gamma^{\rm int}} &= (u_{\rm out}-u_{\rm int})\big|_{\gamma_m^{\rm int}} = (u_m - u),\\
\{u\}\big|_{\gamma_m^{\rm int}} &= \left(\frac{u_{\rm out}+u_{\rm int}}{2}\right) = \left(\frac{u_m+u}{2}\right)_{\gamma_m^{\rm int}},\\
[u]_{\partial\Omega_{\rm int}\setminus\Gamma^{\rm int}} &= (u_{\rm out}-u_{\rm int})\big|_{\partial\Omega_{\rm int}\setminus\Gamma^{\rm int}} = (0-u),\\
\{u\}\big|_{\partial\Omega_{\rm int}\setminus\Gamma^{\rm int}} &= \left(\frac{0+u_{\rm in}}{2}\right)\Bigg|_{\partial\Omega_{\rm int}\setminus\Gamma^{\rm int}}.
\end{aligned}$$

The boundary form of the operator $\frac{\hbar^2}{2m_0}\mathcal{L}^* = -\frac{\hbar^2}{2m*}\triangle + V(x,z)$, without any boundary conditions on $\Gamma^{\rm int}$, on the network $\Omega = \Omega_{\rm int}\cup\Omega_{\rm out}$ is calculated via standard integration by parts. It is convenient to present the boundary form as a function of the jumps $[u] = (u_{\rm out}-u_{\rm int})$ and the mean values $\{u\} = \dfrac{u_{\rm out}+u_{\rm int}}{2}$ of the spinors and their weighted normal derivatives

$$\begin{aligned}
\left[\frac{\partial u}{\partial n}\right] &:= \frac{1}{m^{\|}}\,\frac{\partial u_{\rm out}}{\partial n} - \frac{1}{m^*}\,\frac{\partial u_{\rm int}}{\partial n},\\
\left\{\frac{\partial u_s}{\partial n}\right\}\Bigg|_{\gamma_s} &:= \frac{1}{2}\left\{\frac{1}{m^{\|}}\,\frac{\partial u_{\rm out}}{\partial n} + \frac{1}{m^*}\,\frac{\partial u_{\rm int}}{\partial n}\right\}.
\end{aligned}$$

In particular on $\partial\Omega_{\rm int}\setminus\Gamma^{\rm int}$ we just have $[u] := -u_{\rm int}, \{u\} = \dfrac{u_{\rm int}}{2}$ and

$$\left[\frac{\partial u}{\partial n}\right]\Bigg|_{\partial\Omega_{\rm int}\setminus\Gamma^{\rm int}} := -\frac{1}{m^*}\,\frac{\partial u_{\rm int}}{\partial n},\quad \left\{\frac{\partial u_m}{\partial n}\right\}\Bigg|_{\partial\Omega_{\rm int}\setminus\Gamma^{\rm int}} := -\frac{1}{2}\,\frac{1}{m^*}\,\frac{\partial u_{\rm int}}{\partial n}.$$

Then

$$\begin{aligned}\mathcal{J}_{\mathcal{L}^*} &= \frac{\hbar^2}{2m_0}\langle \mathcal{L}^* u,\, v\rangle - \frac{\hbar^2}{2m_0}\langle u,\, \mathcal{L}^* v\rangle \\ &= \hbar^2 \int_{\partial\Omega_{\rm int}} \left(\left[\frac{\partial u}{\partial n}\right] \{v\}^+ - \{u\} \left[\frac{\partial v}{\partial n}\right]^+ \right) d\gamma \\ &\quad + \hbar^2 \int_{\partial\Omega_{\rm int}} \left(\left\{\frac{\partial u}{\partial n}\right\} [v]^+ - [u] \left\{\frac{\partial v}{\partial n}\right\}^+ \right) d\gamma. \end{aligned} \tag{3.1}$$

We need also the boundary form of the Rashba Hamiltonian. We assume that p_x, p_z are just formal differentiations $i\,\hbar\,\frac{\partial}{\partial x}$, $i\,\hbar\,\frac{\partial}{\partial z}$, respectively. Then on the pair of smooth spinors u, v we have:

$$\begin{aligned}\mathcal{J}_R(u,v) &= \alpha \int_{\Omega_{\rm int}} \left(\sigma_z p_x u v^+ - \sigma_x p_z u v^+\right) dm - \alpha \int_{\Omega_{\rm int}} \left(u \sigma_z p_x v^+ - u \sigma_x p_z v^+\right) dm \\ &= i\hbar\alpha \int_{\partial\Omega_{\rm int}} \left[\cos n_x\, \sigma_z - \cos n_z\, \sigma_x\right] u v^+ d\gamma \\ &= i\hbar\alpha \int_{\partial\Omega_{\rm int}} [\sigma,\, n]_y\, u v^+ d\gamma. \end{aligned} \tag{3.2}$$

The boundary form of the operator $\frac{\hbar^2}{2m_0}\mathcal{L}_R = \frac{\hbar^2}{2m_0}\mathcal{L} + H_R$ on the whole network without any conditions on the boundary and Γ is presented as a sum of forms (3.2), (3.1):

$$\begin{aligned}&\mathcal{J}_{\mathcal{L}^*}(u,v) \\ &= \frac{\hbar^2}{2m*} \int_{\partial\Omega_{\rm int}\setminus\Gamma} \left[u \frac{\partial v^+}{\partial n} - \frac{\partial u}{\partial n}\, v^+ \right] d\gamma \\ &= \int_{\partial\Omega_{in}\setminus\Gamma} u \left(\frac{\hbar^2}{2m^*}\frac{\partial v}{\partial n} - \frac{i\alpha\hbar}{2}[\sigma,n]_y v \right)^+ - \left(\frac{\hbar^2}{2m^*}\frac{\partial u}{\partial n} - \frac{i\alpha\hbar}{2}[\sigma,n]_y u \right) v^+ d\gamma \\ &\quad + \int_\Gamma u \left(\frac{\hbar^2}{2m^*}\frac{\partial v}{\partial n} - \frac{i\alpha\hbar}{2}[\sigma,n]_y v \right)^+ - \left(\frac{\hbar^2}{2m^*}\frac{\partial u}{\partial n} - \frac{i\alpha\hbar}{2}[\sigma,n]_y u \right) v^+ d\gamma \\ &\quad + \hbar^2 \int_\Gamma \left(\left[\frac{\partial u}{\partial n}\right] \{v\}^+ - \{u\} \left[\frac{\partial v}{\partial n}\right]^+ \right) d\gamma \\ &\quad + \hbar^2 \int_\Gamma \left(\left\{\frac{\partial u}{\partial n}\right\} [v^+] - [u] \left\{\frac{\partial v^+}{\partial n}\right\} \right) d\gamma. \end{aligned} \tag{3.3}$$

We proceed assuming that the wave functions are continuous on the network and fulfill Dirichlet boundary conditions on $\partial\Omega$. Then $[u]\Big|_{\Gamma^{\rm int}} = 0$, $\{u\}\Big|_{\Gamma^{\rm int}_{-}} = u_{\rm int}$, hence the sum of last two integrals in the previous formula is reduced via replacement of $\{u\}$ by u to the integral

$$\hbar^2 \int_{\Gamma^{\rm int}} \left(\left[\frac{\partial u}{\partial n}\right] v^+ - u \left[\frac{\partial v}{\partial n}\right]^+ \right) d\gamma,$$

which can be joined with the boundary form of the Rashba Hamiltonian. Then one can see that the boundary form $\mathcal{J}_{\mathcal{L}_R^*}(u,v)$ vanishes if the Dirichlet boundary conditions are imposed on u, v on $\partial\Omega$ and the Rashba matching boundary conditions on $\Gamma^{\rm int}$:

$$\begin{aligned} &\left(\hbar^2 \left[\frac{\partial u}{\partial n}\right] + \frac{i\alpha\hbar}{2}\,[\sigma,\, n]_y\, u_{\rm int}\right)\Bigg|_{\Gamma^{\rm int}} \\ &\quad = \left(\frac{\hbar}{m^{\|}}\,\frac{\partial u_{\rm out}}{\partial n} - \frac{\hbar}{m^*}\,\frac{\partial u_{in}}{\partial n} + \frac{i\alpha}{2}\,[\sigma,\, n]_y\, u_{\rm int}\right)\Bigg|_{\Gamma^{\rm int}} = 0. \end{aligned} \tag{3.4}$$

The Schrödinger operator $\mathcal{L} + H_R$, with Dirichlet boundary conditions on $\partial\Omega$ and the matching boundary condition (3.4) on $\Gamma_{\rm int}$, is self-adjoint in $L_2(\Omega)$.

Definition 3.1. *The operator $\mathcal{L}_R := \mathcal{L} + H_R$ will play a role of full Hamiltonian of an electron on the Quantum network Ω.*

In line with $\mathcal{L}_R$ we consider the operator L_R defined in $L_2(\Omega_{\rm int})$ by the same potential and Rashba Hamiltonian, with Dirichlet boundary condition on the whole boundary $\partial\Omega_{\rm int}$, including $\Gamma^{\rm int}$. We use the geometrical scaling of the spectral parameter $E \to \frac{2m_0 E}{\hbar^2} := \lambda$ and the corresponding scaling of the Schrödinger operators:

$$\frac{\hbar^2}{2m_0}\, L_R u = -\frac{\hbar^2}{2m*}\, \triangle\, u + V(x,z)u + \alpha[\sigma_z\ p_x - \sigma_x\ p_z]u, \quad u|_{\partial\Omega_{\rm int}} = 0. \tag{3.5}$$

The operator $\frac{\hbar^2}{2m_0} L_R$ will play the role of the Hamiltonian of an electron on the quantum dot $\Omega_{\rm int}$. Similar self-adjoint operator on the extended quantum well $\Omega^{\varepsilon}_{\rm int}$ will be denoted by $L^{\varepsilon}_{\rm int}$.

Both operators L_R and $L^{\varepsilon}_{\rm int}$ have discrete spectrum. The eigenvalues and eigenvectors of L_R can be easily computed with a help of standard programs (MATLAB, FEMLAB), and then the eigenvalues of the corresponding operator $L^{\varepsilon}_{\rm int}$ on the extended quantum well can be obtained as small perturbations of them.

We are able to prove, that the solution u of the problem boundary problem for the Schrödinger equation in $\Omega_{\rm int}$ with boundary data on $\Gamma^{\rm int}$ exists, is unique and represented via Poisson map $P_{\rm int}$ of L_R:

$$u = P_{\rm int} u_{\Gamma^{\rm int}_-}\ (x) = \int_{\Gamma^{\rm int}_-} \left[-\frac{1}{\mu^*}\frac{\partial}{\partial n_\xi} + \frac{i\alpha\, m_0}{2\hbar}\,[\sigma,\, n]_y\right] G^{L_R}(x,\xi,\lambda)\ \ u_\Gamma(\xi) d\Gamma_\xi. \tag{3.6}$$

We also connect with the above Dirichlet problem the corresponding Dirichlet-to-Robin map $\mathcal{DR}$. Using the W_2^2-smoothness of the solution of the problem with the boundary data $u_\Gamma \in W_2^{3/2}$ we conclude that the normal current of it $\frac{\partial u}{\partial n}$ on the inner side Γ_- of the bottom sections exists for regular λ and belongs to $W_2^{1/2}(\Gamma)$.

Definition 3.2. For the boundary data $u_{\Gamma^{\rm int}}$ on the inner side $\Gamma_-^{\rm int}$ of the bottom sections we define the Dirichlet-to-Robin map $\mathcal{DR}$ of L_R as the normal current in the outward direction on $\Gamma_-^{\rm int}$, with the Rashba term taken into account,

$$\mathcal{D}_n^R u = \left[-\frac{1}{\mu^*}\frac{\partial}{\partial n_\xi} + \frac{i\alpha\, m_0}{2\hbar}\,[\sigma,\, n]_y\right] u\Big|_{\Gamma_-^{\rm int}} \tag{3.7}$$

for the corresponding solution u of the above boundary problem with the boundary data $u_{\rm int}$ on the inner side $\Gamma_-^{\rm int}$ of $\Gamma_-^{\rm int}$. Then we define the Dirichlet-to-Robin map as

$$\mathcal{DR}\; u_\Gamma = P_+\left[\frac{1}{\mu^*}\frac{\partial}{\partial n} - \frac{i\alpha\, m_0}{2\hbar}\,[\sigma,\, n]_y\right] u\Big|_{\Gamma_-^{\rm int}}, \quad u_\Gamma \in E_+. \tag{3.8}$$

It is convenient to use a special notation for the differential operations on Γ_-, which appeared in (3.6), (3.7), (3.8)

$$\mathcal{D} = \left[-\frac{1}{\mu^*}\frac{\partial}{\partial n} + \frac{i\alpha\, m_0}{2\hbar}\,[\sigma,\, n]_y\right]. \tag{3.9}$$

Then we obtain the standard expressions for the kernels of the Poisson map and Dirichlet-to-Robin map of L_R in terms of $\mathcal{D}$:

$$\begin{aligned} P_R(x,\gamma) &= \mathcal{D}G^{L_R}(x,\gamma)P_+\Big|_{\Gamma_-^{\rm int}}, \\ \mathcal{DR}^{\rm int}(\gamma,\gamma') &= -P_+\mathcal{D}\Big|_\gamma \mathcal{D}\Big|_{\gamma'} G^L(\gamma,\gamma')P_+\Big|_{\gamma\in\Gamma_-^{\rm int}}\Big|_{\gamma'\in\Gamma_-^{\rm int}}. \end{aligned} \tag{3.10}$$

The generalized kernel $\mathcal{DR}^{\rm int}(\gamma,\gamma')$ is represented by the the spectral series

$$\mathcal{DR}^{\rm int}(\gamma,\gamma') = \sum_l \frac{\mathcal{D}\varphi_l\rangle\,\langle\mathcal{D}\varphi_l}{\lambda-\lambda_l}. \tag{3.11}$$

Note that due to Dirichlet boundary conditions for the eigenfunctions φ_l in (3.11) the Rashba term in $\mathcal{D}$ does not contribute to the result on $\Gamma^{\rm int}$:

$$\mathcal{D}\varphi_l\Big|_{\Gamma^{\rm int}} = -\frac{1}{\mu^*}\frac{\partial\varphi_l}{\partial n}.$$

Though this series is divergent, it can be transformed, with use of Hilbert identity, into an uniformly convergent series; see, for instance [30]. This series permits to construct a rational approximation for DR-map and calculate the corresponding approximation for the scattering matrix.

To calculate the scattering matrix in the next section, we need the Dirichlet-to-Neumann of an *intermediate Hamiltonian*, see next section. It can't be calculated based on standard programs, but can be also obtained from the spectral data of L_R and $L_{\rm int}^\varepsilon$ based on an appropriate perturbation procedure, see Sect. 5.

4. Scattering matrix via Intermediate Hamiltonian

The dynamics of an electron on the quantum network on the quantum dot and extended quantum dot are defined by spectral properties of $\mathcal{L}_R$, $L_{\rm int}$ and $L^{\varepsilon}_{\rm int}$ respectively. In our situation the role of the unperturbed Hamiltonian plays the orthogonal sum of the Schrödinger operator on the wires ω_m(in local coordinates)

$$\frac{\hbar^2}{2m_0} L_{\rm out} u_{\rm out} = -\frac{\hbar^2}{2m^{\parallel}} \frac{d^2 u_s}{dx^2} - \frac{\hbar^2}{2m^{\perp}} \frac{d^2 u_s}{dy^2}, \quad u_{\rm out} = \{u_s\}\Big|_{s=1,2,3}, \ u_s\Big|_{\partial\omega_s} = 0, \tag{4.1}$$

and $L^{\varepsilon}_{\rm int}$, and the role of the perturbed operator is played by $\mathcal{L}_R$. The operator $\mathcal{L}_R$ is obtained from $L^{\varepsilon}_{\rm int}$ via attachment of the wires ω_m, which is rather a strong perturbation of the operator with continuous spectrum:

$$\frac{\hbar^2}{2m_0} L^{\varepsilon}_{\rm int} \oplus \frac{\hbar^2}{2m_0} L_{\rm out} \longrightarrow \frac{\hbar^2}{2m_0} \mathcal{L}_R$$

Though physically it is clear that this strong perturbation causes just transformation of the standing waves in the quantum dot into resonance states, due to irradiation of energy into the open channels of the wires, the corresponding mathematics is not yet properly developed. In particular, the analytic perturbation technique for operators with continuous spectrum does not permit to compute the radius of convergence of the perturbation series in spectral terms. Poincare anticipated in [27] that in case of operators with continuous spectrum, the resonances (instead of eigenvalues) should play a role in analytic perturbation procedure. Prigogine attempted to realize the hint by Poincaré, suggesting the idea of "intermediate operator", see [28, 29], and the two-steps analytic perturbation procedure:

$$L^{\varepsilon}_{\rm int} \oplus L_{\rm out} \longrightarrow \mathcal{L}_{\rm interm} \longrightarrow \mathcal{L}_R. \tag{4.2}$$

Prigogine expected that the analytic perturbation procedure is convergent on the second step and attempted to construct $\mathcal{L}_{\rm interm}$ as a function of $L^{\varepsilon}_{\rm int} \oplus L_{\rm out}$. Eventually the idea was abandoned, because it became clear, that the intermediate operator with expected properties does not exist.

In our paper [26] we suggested a modification of the idea of Prigogine, replacing Prigogine's Intermediate Operator by a *finite-dimensional perturbation* of the perturbed operator $\mathcal{L}_R$. This perturbation is introduced via construction a semi-transparent wall on Γ which disrupts the connection between the quantum dot and open channels in the wires, see Appendix below. After splitting off the trivial part in open channels in the n wire we obtain the intermediate Hamiltonian $L_{\rm interm}$ with continuous spectrum beginning from the lowest threshold situated above the Fermi level E_F in the wires. The resonance eigenvalues $\lambda_n^{\rm interm} \approx \frac{2m_0}{\hbar^2} E_F$ of $L_{\rm interm}$ can be calculated based on an analytic perturbation procedure for the *discrete spectrum* of operators $L^{\varepsilon}_{\rm int}$, $L_{\rm interm}$. On the second step of (4.2), we just match the scattering Ansatz in the wires to the square-integrable solution of the homogeneous intermediate equation. This gives an explicit formula for the Scattering matrix of $\mathcal{L}_R$ in terms of the Dirichlet-to-Neumann map of the intermediate Hamiltonian.

The role of a Hamiltonian of a single electron on the network $\Omega = \Omega_{\rm int} \cup \Omega_1 \cup \Omega_2 \cup \Omega_3$ plays the perturbed operator $\mathcal{L}_R$ in $L_2(\Omega)$ defined by the above Schrödinger differential expressions on the extended wires Ω_m and on the well $\Omega_{\rm int}$, the Dirichlet boundary condition $\partial\Omega$ and matching conditions on the boundary $\Gamma^{\rm out} = \cup_m \gamma_m^{\rm out}$ of the wires and the well:

$$[u_{\rm int} - u_m]\Big|_{\gamma_m^{\rm int}} = 0, \quad \frac{\hbar^2}{2m^*}\frac{\partial u_{\rm int}}{\partial n} - \frac{\hbar^2}{2m^{\|}}\frac{\partial u_m}{\partial n} - \frac{i\alpha\hbar}{2}\,[\sigma,\, n]_y\, u_{\rm int}\Big|_{\gamma_m^{\rm int}} = 0, \quad (4.3)$$

which take into account the spin-orbital interaction inside the well.

The Schrödinger operator $\mathcal{L}$ on the network with the above boundary conditions (4.3) is self-adjoint. Our final aim is to calculate the Scattering matrix of this operator with respect to the non-perturbed operator with zero boundary conditions separating the wires from the well. We will fulfill this program based on an intermediate Hamiltonian which may be defined in $L_2(\Omega)$ by slightly altered matching conditions imposed onto elements from the domain of $\mathcal{L}_R$ on $\Gamma^{\rm out}$.

Definition 4.1. Let us consider the cross-section eigenfunctions of the wires $e_{s,n} = \sqrt{\frac{2}{\delta}}\sin\frac{\pi n y}{\delta}$, $n = 1, 2, 3, \dots$, $0 < y < \delta$, $s = 1, 2, 3$ (in local coordinates). Assume that the Fermi level E_F in the wires lies on the first spectral band $\frac{\pi^2}{\delta^2} < E_F\,\frac{2m^\perp}{\hbar^2} < 4\,\frac{\pi^2}{\delta^2}$, hereafter we may assume $E_F = \frac{5}{2}\frac{\hbar^2}{2m^\perp}\frac{\pi^2}{\delta^2}$. Denote by E_+ the linear hull in $L_2(\Gamma^{\rm out})$ of all cross-section eigenvectors of open channels $e_{s,1} = \sqrt{\frac{2}{\delta}}\sin\frac{\pi y}{\delta}$, $0 < y < \delta$, $s = 1, 2, 3$. Similarly we introduce the linear hull E_- of all cross-section eigenfunctions $e_{s,n} = \sqrt{\frac{2}{\delta}}\sin\frac{\pi n y}{\delta}$, $0 < y < \delta$, $s = 1, 2, 3, n = 2, 3, \dots$, of the closed channels. Hereafter we call $E_\pm$ the entrance subspaces of the open and closed channels respectively. Elements of the entrance subspaces we call entrance vectors. We also introduce the corresponding projections $P_\pm$ in $L_2(\Gamma) := E$ as orthogonal sums of corresponding orthogonal projections $P_+^s = e_{1,s}\rangle\,\langle e_{1,s}$, $s = 1, 2, 3, \dots$, onto the orthogonal basis of the entrance vectors $e_{1,s}$, $s = 1, 2, 3$ in E_+, and by P_- the complementary projection in $L_2(\Gamma) : I = P_+ + P_-$. We also introduce the channel spaces $E_\pm \times L_2(R_+) := \mathcal{H}_\pm$.

The channel spaces $\mathcal{H}_\pm$ reduce the operator $L_{\rm out}$ defined by (4.1). The role of the unperturbed operator in the scattering problem on the first spectral band $\Delta_F = \left[\frac{2m^\perp}{\hbar^2}\frac{\pi^2}{\delta^2},\ 4\,\frac{2m^\perp}{\hbar^2}\frac{\pi^2}{\delta^2}\right]$ is played by

$$\mathcal{L}_{\rm out}\Big|_{\mathcal{H}_+} := \frac{\hbar^2}{2m_0} l_F = -\frac{\hbar^2}{2m_0} \oplus \sum_{s=1}^{3} l_s$$

where each of operators $l_s = l \times P_+^s$ is defined by the Dirichlet boundary condition at $x_s = x = 0$ and by the differential expression, in the first channel, $n = 1$:

$$l_{s,1} = \frac{1}{\mu^{\|}} \frac{d^2}{dx^2} - \frac{1}{\mu^{\perp}} \frac{\pi^2}{\delta^2}, \quad s = 1, 2, 3, \tag{4.4}$$

with $\mu^{\|} = m^{\|} m_0^{-1}$, $\mu^{\perp} = m^{\perp} m_0^{-1}$. The operator l_F is obtained from $\mathcal{L}_R$ via submitting the elements of $D(\mathcal{L}_R)$ to the additional boundary condition (4.6), (4.7) on $\Gamma = \cup_{s=1}^3 \omega_s$ in open and closed channels respectively. Note that the boundary term $\frac{i\alpha}{2} [\sigma, n]_y$ arising from the Rashba Hamiltonian commutes with projection onto the entrance vectors of the channels. We obtain a self-adjoint split operator $\frac{2m_0}{\hbar^2} \mathcal{L}_F = L_F \oplus l_F$,

$$\begin{aligned} L_F u_{\text{in}} &:= L_{\text{int}} u_{\text{int}} = -\frac{1}{\mu^*} \triangle u_{\text{int}} + \frac{i\alpha m_0}{\hbar} [\sigma, \nabla]_y u_{\text{int}}, \quad u_{\text{int}} \in W_2^2(\Omega_{\text{int}}), \\ L_F u_{\text{out}} &:= l_{\text{out}} u_{\text{out}} = -\frac{1}{\mu^{\|}} \frac{d^2 u_{\text{out}}}{dx^2} + \frac{1}{\mu^{\perp}} \sum_{s,n,-} \frac{n^2\pi^2}{\delta^2} P_{s,n} u_{\text{out}}, \quad u_{\text{out}} \in \mathcal{H}_-, \end{aligned} \tag{4.5}$$

where the summation in $\sum_{s,n,-}$ is extended over all closed channels, and

$$l_F u_{\text{out}} := l_{\text{out}} u_{\text{out}} = -\frac{1}{\mu^{\|}} \frac{d^2 u_{\text{out}}}{dx^2} + \frac{1}{\mu^{\perp}} \sum_{s,n,+} \frac{\pi^2}{\delta^2} P_{s,n,+} u_{\text{out}}, \quad u_{\text{out}} \in \mathcal{H}_+,$$

where summation extended over the open channels $n = 1, s = 1, 2, 3$. We impose on $u = (u_{\text{int}}, u_{\text{out}})$ from the domain of L_F the partial Dirichlet boundary conditions on Γ^{out} in open channels :

$$P_+ u_s\big|_\Gamma = 0, \quad P_+ u_{\text{int}}\big|_{\Gamma^{\text{out}}} = 0, \tag{4.6}$$

and partial matching conditions in closed channels:

$$P_- [u_{\text{int}} - u_{\text{out}}]\big|_{\Gamma^{\text{out}}} = 0.$$

$$\frac{1}{\mu^*} P_- \frac{\partial u_{\text{int}}}{\partial n} - \frac{1}{\mu^{\|}} P_- \frac{\partial u_{\text{out}}}{\partial n} - \frac{i\alpha\, m_0}{2\hbar} [\sigma, n]_y P_- u_{\text{int}}\big|_{\Gamma^{\text{out}}} = 0. \tag{4.7}$$

Note that due to the above assumption, the Rashba term vanishes on the link, hence it is absent on Γ^{out} in (4.7). Hence the above boundary condition is reduced to

$$\frac{1}{\mu^*} P_- \frac{\partial u_{\text{int}}}{\partial n} - \frac{1}{\mu^{\|}} P_- \frac{\partial u_{\text{out}}}{\partial n}\Big|_{\Gamma^{\text{out}}} = 0. \tag{4.8}$$

Spectral properties of the operator $\frac{2m_0}{\hbar^2}\mathcal{L}$ with respect to the scaled "geometrical" spectral parameter $\lambda = 2m_0 E \hbar^{-2}$ are described in Sect. 6, see Theorem 6.1.

Definition 4.2. The operator L_F is considered hereafter as an intermediate Hamiltonian.

The intermediate Hamiltonian is self-adjoint in $L_2(\Omega) \ominus \mathcal{H}_+ := \mathcal{H}^{\perp}$ on the domain of elements $\{u\}$ from $W_2^1(\Omega)$ which are locally smooth, $u \in W_2^2(\Omega_{\text{int}}) \cap W_2^2(\Omega_{\text{out}})$ and fulfill the partial Dirichlet boundary condition on the inner side of Γ in the open channel and the partial matching boundary condition in closed channels. Denote by $\lambda_{\rm min}$ the minimal threshold of closed channels

$$\min_{\frac{\pi^2 n^2}{\delta^2} > \frac{2m_0}{\hbar^2} E_F} \frac{\pi^2 n^2}{\delta^2} := \lambda_{\rm min}$$

The absolutely continuous spectrum $\sigma_a(L_F)$ fills the interval $\left[\lambda^F_{\rm min}, \infty\right)$, with varying multiplicity. There may be only a finite number of eigenvalues of L_F below $\lambda^F_{\rm min}$. Those of them which are situated on the conductivity band Δ_F between $\lambda_{\rm min}$ and the maximal threshold of open channels

$$\lambda_{\rm max} := \max_{\frac{\pi^2 n^2}{\delta^2} < \frac{2m_0}{\hbar^2} E_F} \frac{\pi^2 n^2}{\delta^2}$$

are called resonance eigenvalues of L_F. In our case, according to above assumption $\lambda_{\rm max} = \pi^2\delta^{-2}$, $\lambda_{\rm min} = 4\pi^2\delta^{-2}$. We assume that the resolvent of the intermediate Hamiltonian $[L_F - \lambda I]^{-1}$ is constructed. The restriction

$$P_{L_2(\Omega)\ominus\mathcal{H}_+}[L_F - \lambda I]^{-1} P_{L_2(\Omega_{\rm int})}$$

has a kernel G^F which is obtained by a finite-dimensional perturbation of the Green function $G^{\mathcal{L}_R}$.

To construct the scattering matrix we have to solve the intermediate Dirichlet problem:

Definition 4.3. Consider the solution $u \in \mathcal{H}_+^\perp$ of the Schrödinger equation with the spectral parameter from the resolvent set of L_F,

$$L^\varepsilon_{\rm int}\, u_{\rm int} - \lambda\, u_{\rm int} = 0, \quad l_{\rm out}\, u_{\rm out} - \lambda\, u_{\rm out} = 0,$$

with $(u_{\rm int}, u_{\rm out}) := u \in W_2^1(\Omega) \cap W_2^2(\Omega_{\rm int}) \cap W_2^2(\Omega_{\rm out})$. If u satisfies the condition $u\big|_{\Gamma^{\rm out}_-} = u_{\Gamma^{\rm out}} \in E_+$ on the inner side $\Gamma^{\rm out}_-$ of $\Gamma^{\rm out}$ and the matching boundary conditions (4.7) imposed on the jump of u, $\frac{\partial u}{\partial n}$ on $\Gamma^{\rm out}$, then we call u the solution of the intermediate boundary problem with the boundary data $u_{\Gamma^{\rm out}}$.

Due to vanishing of the Rashba term on $\Gamma^{\rm out}$ the formula (3.6) for the Poisson map of the intermediate Hamiltonian is reduced for on $\Gamma^{\rm out}$ to

$$u = P_F u_\Gamma\ (x) = \int_{\Gamma^{\rm out}} \left[-\frac{1}{\mu^*}\frac{\partial}{\partial n_\xi}\right] G^{L_F}(x,\xi,\lambda)\ u_\Gamma(\xi) d\Gamma_\xi. \tag{4.9}$$

The corresponding DN-map is calculated as:

$$\begin{aligned} \mathcal{DN}^F u &= \frac{1}{\mu^*}\frac{\partial P_F u_\Gamma}{\partial n}(x)\big|_{\Gamma^{\rm out}_-} \\ &= \int_{\Gamma^{\rm out}} \left[-\left(\frac{1}{\mu^*}\right)^2 \frac{\partial^2}{\partial n_x \partial n_\xi}\right] G^{L_F}(x,\xi,\lambda)\ u_\Gamma(\xi) d\Gamma_\xi\,\big|_{\Gamma^{\rm out}_-}. \end{aligned} \tag{4.10}$$

Based on (4.10), we obtain first an exact explicit expression for the scattering matrix:

Theorem 4.4. *Let K_+ be the exponent of oscillating solutions of the Schrödinger equation in the open channel which admit analytic bounded continuation onto the physical sheet of the spectral variable: $K_+ = \sqrt{\mu^{\|}}\sqrt{\lambda - \frac{\pi^2}{\mu^{\perp}\delta^2}} > 0$. Then*

$$S(\lambda) = \frac{iK_+/\mu^{\|} + \mathcal{DN}^F}{iK_+/\mu^{\|} - \mathcal{DN}^F}. \tag{4.11}$$

Proof. Note that the matching conditions in closed channels are fulfilled for solution of their intermediate boundary problem. Hence we need to verify only matching conditions in open channels. This gives, with the scattering Ansatz in open channels $\Psi_+ = e^{iK_+x}\nu_+ + e^{-iK_+x}S\nu_+$:

$$-\mathcal{DN}^F\left[\nu_+ + S\nu_+\right]\Big|_{\Gamma_+} = -\frac{1}{\mu^{\|}}\frac{\partial}{\partial n}\Psi_{\text{out}}\Big|_{\Gamma_+} = -iK_+/\mu^{\|}\left[\nu_+ - S\nu_+\right]\Big|_{\Gamma_+}. \tag{4.12}$$

Note that the matrix-functions $\mathcal{DN}^F, |, K_+$ are Hermitian on real axis of the spectral parameter λ, below $\lambda^F_{\min}$. Then the scattering matrix can be obtained from (4.12) in announced form (4.11). □

Unfortunately, DN-map of the intermediate Hamiltonian can't be obtained based on standard software. We will compute it via analytic perturbation procedure based on the DN-map of the Schrödinger operator L_R on the extended quantum well $\Omega^{\delta}_{\text{int}}$, including small cut-offs of the wires, with Dirichlet condition on the boundary.

5. Re-normalization of spectral data of the Schrödinger operator on the quantum well

In this section we develop a two-steps analytic perturbation procedure aimed on calculation of the transmission coefficient across the quantum well. Recall, that the Rashba term is included into the Schrödinger operator on the well, but absent on the wires. In this paper we just assume that the Rashba term vanishes abruptly, by jump at the boundary of the quantum well Ω_{int}. We include in our analysis the case when the wires enter the well non-orthogonally. Our analysis of the zone of contact permits to consider also models with strictly intrinsic Rashba terms, fading at the boundary of the well.

The standard approach to the calculation of the scattering matrix is based on matching the full scattering Ansatz in the wires

$$\Psi_{\text{out}} = e^{iK_+x}\nu_+ + e^{-iK_+x}S\nu_+ + e^{-K_-x}s\nu_+$$

containing the exponentially decreasing component $e^{-K_-x}s\nu_+$ in closed channels, to the smooth solution of the corresponding homogeneous Schrödinger equation on the extended quantum well.

Denote by $L^{\varepsilon}_{\text{int}}$ the restriction of the Schrödinger operator $\mathcal{L}_R$ onto $\Omega^{\varepsilon}_{\text{int}}$ with Dirichlet boundary conditions on $\partial\Omega^{\varepsilon}_{\text{int}}$, and consider the corresponding boundary problem with zero boundary condition on $\partial\Omega^{\varepsilon}_{\text{int}}\backslash\Gamma^{\text{out}}_-$ and non-homogeneous

Dirichlet boundary condition on the inner side $\Gamma_-^{\rm out}$ of the union of all bottom sections:

$$u\big|_{\Gamma_-^{\rm out}} = u_{\Gamma_\delta} \in W_2^{3/2}(\Gamma_-^{\rm out}).$$

We consider the normal boundary current of the solution and introduce the corresponding DN-map

$$\mathcal{DN} : u_{\Gamma_\delta} \to \frac{1}{m^*}\frac{\partial u}{\partial n}\bigg|_{\Gamma_-^{\rm out}}.$$

Using $\mathcal{DN}$ we can obtain an explicit expression for the scattering matrix via matching of the scattering Ansatz in the wires to the appropriate solution of the above boundary problem on the extended quantum well. The matching boundary condition at bottom sections Γ with the scaled effective masses

$$[u_0 - u_s]\big|_{\gamma_s^{\rm out}} = 0, \quad \frac{1}{\mu^*}\ \frac{\partial u_0}{\partial n} - \frac{1}{m^{\|}}\ \frac{\partial u_s}{\partial n} = 0, \tag{5.1}$$

gives a linear system for the boundary values u, $\frac{\partial u}{\partial n}$ of the scattered wave on the inner part $\Gamma_-^{\rm out}$ of $\Gamma^{\rm out}$:

$$u = \nu + S\nu + s\nu$$
$$\mathcal{DN}u = i\frac{1}{\mu^{\|}}K_+(\nu - S\nu) - \frac{1}{\mu^{\|}}K_- s\nu.$$

The second equation of the system can be represented in terms of matrix elements of the DN-map $\mathcal{DN}$ of the operator L^D with respect to the orthogonal decomposition $E = E_+ + E_-$

$$\mathcal{DN} = \begin{pmatrix} P_+\mathcal{DN}P_+ & P_+\mathcal{DN}P_- \\ P_-\mathcal{DN}P_+ & P_-\mathcal{DN}P_- \end{pmatrix} := \begin{pmatrix} \mathcal{DN}_{++} & \mathcal{DN}_{+-} \\ \mathcal{DN}_{-+} & \mathcal{DN}_{--} \end{pmatrix}.$$

This implies the following equation for the components $S\nu, s\nu$ of the Scattering Ansatz:

$$\begin{pmatrix} \mathcal{DN}_{++} & \mathcal{DN}_{+-} \\ \mathcal{DN}_{-+} & \mathcal{DN}_{--} \end{pmatrix} \begin{pmatrix} \nu + S\nu \\ s\nu \end{pmatrix} = \begin{pmatrix} i\frac{1}{\mu^{\|}}K_+(\nu - S\nu) \\ -\frac{1}{\mu^{\|}}K_- s\nu \end{pmatrix}.$$

Eliminating from this equation the component of the scattered wave in the closed channels we obtain:

$$\left(\mathcal{DN}_{++} - \mathcal{DN}_{+-}\frac{I}{\mathcal{DN}_{--} + \frac{1}{\mu^{\|}}K_-}\mathcal{DN}_{-+}\right)(\nu + S\nu) = i\frac{1}{\mu^{\|}}K_+\left(\nu - S\nu\right). \tag{5.2}$$

Comparing (5.2) with the above equation (4.11), we see that

$$\mathcal{DN}_{++} - \mathcal{DN}_{+-}\frac{I}{\mathcal{DN}_{--} + \frac{1}{\mu^{\|}}K_-}\mathcal{DN}_{-+} = \mathcal{DN}^F \tag{5.3}$$

everywhere on real axis where the matrix

$$I + S = \frac{2i\frac{1}{\mu^{\|}}K_+}{i\frac{1}{\mu^{\|}}K_+ - \mathcal{DR}^F}$$

is invertible. But

$$(I+S)^{-1} = I - \left(i\frac{1}{\mu^{\|}}K_+\right)^{-1} \mathcal{DN}^F$$

exists on the complement of the spectrum of the intermediate operator. Thus, the following statement is proven:

Theorem 5.1. *The DN-map of the intermediate operator exists on the complement of the spectrum of the intermediate hamiltonian and is represented in terms of the DN-map of the Schrödinger operator L^D on the well as*

$$\mathcal{DN}^F = \mathcal{DN}_{++} - \mathcal{DN}_{+-}\frac{I}{\mathcal{DN}_{--} + \frac{1}{\mu^{\|}}K_-}\mathcal{DN}_{-+}. \tag{5.4}$$

Note that the expression in the right side may have singularities at the spectrum of the Schrödinger operator on the quantum well-because of matrix elements $\mathcal{DN}_{\pm,\pm}$ and singularities caused by the zeros of the denominator $\mathcal{DN}_{--} + \frac{1}{\mu^{\|}}K_-$. We are able to show, that for shrinking or relatively thin quantum networks the singularities of the expression in the right-hand side of (5.4) at the eigenvalues of the Schrödinger operator on the quantum well cancel each other, and the singularities at zeros of the denominator $\mathcal{DN}_{--} + \frac{1}{\mu^{\|}}K_-$ define the spectrum of the intermediate Hamiltonian.

Definition 5.2. We will keep the quantum well unchanged, but consider a special shrinking of the extended wires (the wires and the cut-offs), assuming that the Fermi level Λ is constant, and the constant potential is added on the extended wires Ω_m shifting the thresholds of the conductivity band

$$\lambda_{\min,\max}(\delta) = \delta^{-2}\lambda^1_{\min,\max} + V_m(\delta)$$

such that the Fermi-level Λ

$$\Lambda = V_m(\delta) + \frac{1}{2\delta^2}\left[\lambda^1_{\min} + \lambda^1_{\max}\right] \tag{5.5}$$

remains constant and is situated in the middle of the conductivity band $\Delta_F = [\lambda_{\max}(\delta),\, \lambda_{\min}(\delta)]$ in the course of shrinking. All geometric details of shrinking wires are supplied by the index δ, to emphasis the role of the shrinking parameter, for instance, we replace now:

$$\Omega^{\varepsilon}_{\text{int}} \longrightarrow \Omega^{\delta}_{\text{int}},$$

We assume that the width of the shrinking wires is defined by the parameter δ as $\delta^1 \times \delta$, where δ^1 is fixed (we may assume that $\delta^1 = 1$), $\lambda^1_{\min,\max}$ are constant in course of shrinking, and $\delta \to 0$. We assume that the potential on the links is changing in course if shrinking the same way as the potential on the wires (5.5).

Lemma 5.3. *The size $|\Delta_F| = \lambda_{\min}(\delta) - \lambda_{\max}(\delta)$ of the conductivity band increases when shrinking, $\delta \to 0$, as*

$$|\Delta_F| = \frac{1}{\delta^2}\left[\lambda^1_{\min} - \lambda^1_{\max}\right] \to \infty. \tag{5.6}$$

Proof. Obvious. □

Hereafter we assume that the conductivity band is just the first spectral band $\left[V_m + \frac{\pi^2}{\mu^\perp \delta^2}, V_m + 4\frac{\pi^2}{\mu^\perp \delta^2}\right]$, and the Fermi level lies in the middle of it $\Lambda = V_m + \frac{5}{2}\,\frac{\pi^2}{\delta^2}$. One can derive from (5.3) that the the spectrum of the Schrödinger operator on the links, with the Neumann boundary condition on the side $\gamma^\delta_{\rm int}$ and the Dirichlet boundary condition on other sides, lies above the Fermi level, if certain geometrical condition is satisfied, see the discussion below in this section.

We impose a special geometric conditions on the shape of the links. We formulate this condition for a single wire. Recall, that we already denoted by $\gamma_m^{\rm int}$ the bottom section of the shrinking extended wires in $\Gamma_{\rm int}$, and by $\gamma^{\rm out} \in \Gamma^{\rm out}$ the union of the orthogonal bottom section of the wires ω_m. Consider spectral problem for the Schrödinger operator L^N_δ on the shrinking trapezial link Ω^δ with the Neumann boundary condition on the "skew" side $\gamma^{\rm int}$ and Dirichlet boundary conditions on the other sides of Ω^δ. Denote by λ^δ the minimal eigenvalue of L^N_δ.

Lemma 5.4. *If the condition*

$$\lambda^\delta > \Lambda \tag{5.7}$$

is fulfilled then the restriction $\mathcal{DN}_{\rm int,int}(\lambda)$ *of the DN-map of the link onto* $\Gamma^{\rm int}$ *is an invertible operator when* λ *is in a small neighborhood of* Λ*.*

Proof. Denote by G^N_δ the Green function of the operator L^N_δ. The inverse of the restriction of the DN-map of L^δ on $\gamma^{\rm int}$ is defined by the integral operator, see [30]:

$$Qv(x) = \int_{\Gamma^{\rm out}} G^N_\delta(x,\xi,\lambda)v(\xi)d\xi.$$

The integral in the right side exists if the λ is not an eigenvalue of L^N_δ. □

If the condition (5.7) is fulfilled for the Fermi level, then it is fulfilled also in some neighborhood of it. Hereafter we assume that it is fulfilled also for the resonance eigenvalue λ_0 of L^D. In simplest case, when the tensor of effective mass is isotropic, $\mu^\parallel = \mu^\perp = \mu^*$, this condition can be replaced by stronger, but easily verifiable condition for the minimal rectangle $\square_\delta$ which contains the link Ω^δ and it's reflection in $\gamma_{\rm int}$, and is symmetric with respect to reflection in $\gamma^\delta_{\rm int}$. For instance, if the Fermi level Λ lies in the middle of the first spectral band, $\Lambda = 5\pi^2\,\mu^{-1}\delta^{-2}/2 + V_\omega$ this condition is

$$\frac{1}{[\tan\theta + 2\varepsilon]^2} + \frac{1}{[\cos\theta + 2^{-1}\sin^2\theta + \varepsilon\sin\theta]^2} > 5/2.$$

Consider the Schrödinger operator L^δ on the link Ω^δ with Dirichlet boundary conditions. Denote by DN^δ the restriction of the DN-map of L^δ onto the sides $\gamma^{\rm in}, \gamma^{\rm out}$, and introduce the orthogonal decomposition of the restriction with respect to the $L_2(\gamma^{in}) \oplus L_2(\gamma^{\rm out})$

$$DN^\delta = \begin{pmatrix} DN^\delta_{\rm out,out} & DN^\delta_{\rm out,int} \\ DN^\delta_{\rm int,out} & DN^\delta_{\rm int,int} \end{pmatrix}.$$

The following statement gives a link between the DN-map of the Schrödinger operator L_R on the quantum well $\Omega_{\rm int}$ and the DN-map of the operator $L^\delta_{\rm int}$ on the extended quantum well with shrinking links attached.

Theorem 5.5. *The Dirichlet-to-Neumann map of the Schrödinger operator $L^\delta_{\rm int}$ in $L_2(\Omega^\delta_{\rm int})$ with Dirichlet boundary conditions is approximately calculated at the Fermi level as*

$$\begin{aligned}\mathcal{DN}^\delta_{\rm int} \approx\, & DN^\delta_{\rm out,out} - DN^\delta_{\rm out,int}[DN^\delta_{\rm int,int}]^{-1} DN^\delta_{\rm int,out} \\ & + \frac{DN^\delta_{\rm out,in}[DN^\delta_{\rm int,int}]^{-1}\mathcal{D}\varphi_0\rangle\,\langle DN^\delta_{\rm out,in}[DN^\delta_{\rm int,int}]^{-1}\mathcal{D}\varphi_0}{\lambda-\lambda_0+\langle \mathcal{D}\varphi_0, [DN^\delta_{\rm int,int}]^{-1}\mathcal{D}\varphi_0\rangle}.\end{aligned} \tag{5.8}$$

Proof. It is sufficient to prove the statement for a compact domain $\Omega_{\rm int}$ with a single quantum wire ω width δ attached to it on a flat piece $\Gamma^{\rm int}\in\partial\Omega_{\rm int}$ of the boundary. The corresponding link Ω^δ is included into the extended quantum well $\Omega^\delta_{\rm int}=\Omega_{\rm int}\cup\Omega^\delta$.

To calculate the restriction of the DN-map of the Schrödinger operator $L^\delta_{\rm int}$ on $\gamma^\delta_{\rm out}$ we represent the restriction of the DN-map of the link onto $\gamma^\delta_{\rm int}\cup\gamma^\delta_{\rm out}$ in terms of the orthogonal decomposition of $L_2(\gamma^\delta_{\rm int}\cup\gamma^\delta_{\rm out}) = L_2(\gamma^\delta_{\rm int})\oplus L_2(\gamma^\delta_{\rm out})$ as a matrix.

Denote by $\mathcal{DR}_{\rm int}$ the DR map of the operator L_R on the well $\Omega_{\rm int}$, and by $\mathcal{DN}^\delta_{\rm int}$ the DN-map of the operator $L^\delta_{\rm int}$,on the extended well, restricted onto $\gamma^\delta_{\rm out}$. Consider the solution u of the boundary problem on the extended well,

$$L^\delta_{\rm int}u=\lambda u,\quad u\big|_\Gamma = u_\Gamma$$

and denote by $u_{\rm int}$ and $u_{\rm out}$ the data of u on $\gamma^{\rm int}$ and $\gamma_{\rm out}$, respectively. These data are connected by the equation

$$\begin{pmatrix} DN^\delta_{\rm out,out} & DN^\delta_{\rm out,int} \\ DN^\delta_{\rm int,out} & DN^\delta_{\rm int,int}\end{pmatrix}\begin{pmatrix} u_{\rm out} \\ u_{\rm int}\end{pmatrix} = \begin{pmatrix} \mathcal{DN}^\delta_{\rm int}u_{\rm out} \\ -\mathcal{DR}_{\rm int}u_{\rm int}\end{pmatrix}.$$

Solving this equation with respect to $\mathcal{DN}^\delta_{\rm int}u_{\rm out}$ we obtain the explicit expression for $\mathcal{DN}^\delta_{\rm int}$

$$\mathcal{DN}^\delta_{\rm int} = DN^\delta_{\rm out,out} - DN^\delta_{\rm out,int}\frac{I}{DN^\delta_{\rm int,int}+\mathcal{DR}_{\rm int}}DN^\delta_{\rm in,out}. \tag{5.9}$$

The singularities of the whole expression are defined by the zeros of the denominator

$$DN^\delta_{\rm int,int}+\mathcal{DR}_{\rm int} := \mathcal{D}_\delta \tag{5.10}$$

and by singularities of the matrix elements of $\mathcal{DN}^\delta$. Due to condition (5.7), we see that $\mathcal{DN}^\delta_{\rm int,int}(\lambda)$ is invertible at the Fermi level. The Schrödinger operator on the cut-off is homogeneous of degree -2, hence the corresponding DN-map is also homogeneous of degree -1. In particular this means that the inverse of it acts, at regular values of the spectral parameter, from $W_2^{1/2}(\partial\Omega^\varepsilon)$ into $W_2^{3/2}(\partial\Omega^\varepsilon)$ with the norm estimated by const$\cdot\delta$, with an absolute constant, which coincides with the norm of the inverse of the non-scaled cut-off width $\delta = 1$ at the Fermi level Λ. This allows us to represent the restriction onto $\gamma^\delta_{\rm out}$ of the DN-map of $L^\delta_{\rm int}$ as

$$\mathcal{DN}^\delta_{\rm int} = DN^\delta_{\rm out,out} - DN^\delta_{\rm out,in}\frac{I}{I + [DN^\delta_{\rm int,int}]^{-1}\mathcal{DR}_{\rm int}}[DN^\delta_{\rm out,out}]^{-1}DN^\delta_{\rm in,out}. \tag{5.11}$$

We calculate the inverse $[I + [DN^\delta_{\rm out,out}]^{-1}\mathcal{DR}_{\rm int}]^{-1}$ assuming that $\mathcal{DN}_{\rm int}$ is represented near Fermi level $\Lambda \approx \lambda_0$ in form of spectral series (3.11). Taking into account only one resonance polar term $\frac{\mathcal{D}\varphi_0\rangle\,\langle\mathcal{D}\varphi_0}{\lambda-\lambda_0}$ and denoting the remainder by $\mathcal{K}$ we obtain

$$[DN^\delta_{\rm int,int}]^{-1}\mathcal{DR}_{\rm int} = \frac{[DN^\delta_{\rm int,int}]^{-1}\mathcal{D}\varphi_0\rangle\,\langle\mathcal{D}\varphi_0}{\lambda-\lambda_0} + [DN^\delta_{\rm out,out}]^{-1}\mathcal{K}.$$

Both terms in the right side are bounded operators in $W_2^{3/2}(\gamma^\delta_{\rm out})$, and can be extended by continuity onto $L_2(\gamma^\delta_{\rm out})$. The corresponding norm of the second term can be estimated, due to homogeneity of $\mathcal{DN}^\delta_{\rm out,out}$, as

$$\parallel [DN^\delta_{\rm int,int}]^{-1}\mathcal{K}\parallel_2 \leq \delta \parallel [DN^1_{\rm int,int}]^{-1}\mathcal{K}\parallel_2,$$

hence it is small for small δ. Introducing the notations

$$[DN^\delta_{\rm int,int}]^{-1}\mathcal{D}\varphi_0 := \delta\phi'_0, \quad \mathcal{D}\varphi_0 := \phi_0, \quad [DN^\delta_{\rm out,out}]^{-1}\mathcal{K} := \delta\mathcal{K}_1,$$

we notice that construction of the inverse $[I + [DN^\delta_{\rm out,out}]^{-1}\mathcal{DN}_{\rm int}]^{-1}$ requires solving the following equation in $L_2(\gamma^\delta_{\rm out})$:

$$\left(I + \delta\mathcal{K}_1 + \delta\frac{\phi'_0\rangle\,\langle\phi_0}{\lambda-\lambda_0}\right)u = f,$$

$$u = \left[(I+\delta\mathcal{K}_1)^{-1} * + \frac{(I+\delta\mathcal{K}_1)^{-1}\delta\phi'_0\rangle\,\langle\phi_0, (I+\delta\mathcal{K}_1)^{-1}*}{\lambda-\lambda_0+\langle\delta\phi'_0, (I+\delta\mathcal{K}_1)^{-1}\phi_0\rangle}\right]f.$$

Hence the DN-map of $L^\delta_{\rm int}$, restricted onto $\gamma^\delta_{\rm out}$ is represented near resonance as

$$\mathcal{DN}^\delta_{\rm int} = DN^\delta_{\rm out,out} - DN^\delta_{\rm out,int}(I+\delta\mathcal{K}_1)^{-1}[DN^\delta_{\rm int,int}]^{-1}DN^\delta_{\rm int,out} +$$
$$\frac{DN^\delta_{\rm out,in}(I+\delta\mathcal{K}_1)^{-1}[DN^\delta_{\rm int,int}]^{-1}\mathcal{D}\varphi_0\rangle\,\langle DN^\delta_{\rm out,in}(I+\delta\mathcal{K}_1)^{-1}[DN^\delta_{\rm int,int}]^{-1}\mathcal{D}\varphi_0}{\lambda-\lambda_0+\langle\mathcal{D}\varphi_0, (I+\delta\mathcal{K}_1)^{-1}[DN^\delta_{\rm int,int}]^{-1}\mathcal{D}\varphi_0\rangle}. \tag{5.12}$$

Due to presence of $[DN^\delta_{\rm int,int}]^{-1}$ containing the factor δ in the second and third terms in the right side we see that the magnitude of these terms is of the order δ and δ^2, respectively. Similarly, the quadratic form in the denominator of the third term is estimated for small δ as $\langle\mathcal{D}\varphi_0, [DN^\delta_{\rm int,int}]^{-1}\mathcal{D}\varphi_0\rangle \approx \delta{\cdot}{\rm const}$, so

$$\mathcal{DN}^\delta_{\rm int} \approx DN^\delta_{\rm out,out} - DN^\delta_{\rm out,int}[DN^\delta_{\rm int,int}]^{-1}\,DN^\delta_{\rm int,out}$$
$$+\frac{\mathcal{DN}^\delta_{\rm out,in}[DN^\delta_{\rm int,int}]^{-1}\mathcal{D}\varphi_0\rangle\,\langle DN^\delta_{\rm out,int}[DN^\delta_{\rm int,int}]^{-1}\mathcal{D}\varphi_0}{\lambda-\lambda_0+\langle\mathcal{D}\varphi_0, [DN^\delta_{\rm int,int}]^{-1}\mathcal{D}\varphi_0\rangle}, \tag{5.13}$$

completing the proof. □

Note that, due to Dirichlet boundary conditions the Rashba term in $\mathcal{D}$ does not contribute to result, and $\mathcal{D}$ is reduced just to the differentiation $\mathcal{D} = -\frac{1}{m*}\frac{\partial}{\partial n}$.

The approximate expression for the restriction of the DN-map of $L^{\delta}_{\rm int}$ onto $\gamma^{\delta}_{\rm out}$ will be used in course of calculation of the DN-map of the intermediate Hamiltonian.

Now, assuming that the network is thin and the Fermi level is situated in the middle of the first spectral band we calculate approximately the DN-map of the intermediate Hamiltonian L_F, based on (5.4) and (5.11).

We will need more elaborated notations. Let Δ be the sub-interval of the conductivity band $\Delta_F = (\lambda_{\max}, \lambda_{\min})$, centered at the scaled Fermi-level Λ. We assume that the above approximation (5.13) for $\mathcal{DN}^{\delta}_{\rm int}$ is valid on Δ, and $\lambda_0 \in \Delta$ is the resonance eigenvalue of the Schrödinger operator L_R in $L_2(\Omega_{\rm int})$, with zero boundary conditions. According to (5.13) we obtain the resonance eigenvalue of $L^{\delta}_{\rm int}$ as a perturbation of λ_0:

$$\lambda_0^{\delta} \approx \lambda_0 - \langle \mathcal{D}\varphi_0, [DN^{\delta}_{\rm int,int}]^{-1}\mathcal{D}\varphi_0\rangle. \tag{5.14}$$

The corresponding residue $\phi_0\rangle\langle\phi_0$ is constructed based on the eigenvector φ_0 of the operator L_R with Dirichlet boundary condition on $\partial\Omega_{\rm int}$

$$\phi_0 = DN^{\delta}_{\rm out,in}(I+\delta\mathcal{K}_1)^{-1}[DN^{\delta}_{\rm int,int}]^{-1}\mathcal{D}\varphi_0 \approx DN^{\delta}_{\rm out,in}[DN^{\delta}_{\rm int,int}]^{-1}\mathcal{D}\varphi_0. \tag{5.15}$$

Separate the resonance term of (5.13)

$$\frac{\phi_0\rangle\langle\phi_0}{\lambda-\lambda_0^{\delta}} := \mathcal{DN}^{\Delta},$$

and consider the remainder

$$\mathcal{DN}^{\Delta'} = \mathcal{DN} - \mathcal{DN}^{\Delta} := \mathcal{K} : W_2^{3/2}(\Gamma) \to W_2^{1/2}.$$

We will use the decomposition of $L_2(\gamma^{\rm out}) := E$ into the sum of entrance subspaces of open and closed channels: $E = E_+ \oplus E_-$. Represent the DN-map $\mathcal{DN}$ of L^D by the 2×2 matrix with respect to this decomposition

$$\mathcal{DN} = \begin{pmatrix} \mathcal{DN}_{++} & \mathcal{DN}_{+-} \\ \mathcal{DN}_{-+} & \mathcal{DN}_{--} \end{pmatrix}.$$

The matrix elements can be presented as

$$\begin{aligned}
\mathcal{DN}_{++} &= \mathcal{DN}^{\Delta}_{++} + \mathcal{DN}^{\Delta'}_{++} := \mathcal{DN}^{\Delta}_{++} + \mathcal{K}_{++},\\
\mathcal{DN}_{+-} &= \mathcal{DN}^{\Delta}_{+-} + \mathcal{DN}^{\Delta'}_{+-} := \mathcal{DN}^{\Delta}_{+-} + \mathcal{K}_{+-},\\
\mathcal{DN}_{-+} &= \mathcal{DN}^{\Delta}_{-+} + \mathcal{DN}^{\Delta'}_{-+} := \mathcal{DN}^{\Delta}_{+-+} + \mathcal{K}_{-+},\\
\mathcal{DN}_{--} &= \mathcal{DN}^{\Delta}_{--} + \mathcal{DN}^{\Delta'}_{--} := \mathcal{DN}^{\Delta}_{--} + \mathcal{K}_{--}.
\end{aligned}$$

Here $\mathcal{K}_{++}$, $\mathcal{K}_{+-}$, $\mathcal{K}_{--}$ are the matrix elements of the contribution $\mathcal{K}$ to the DN-map from the non-resonance eigenvalues $\lambda_l \in \Delta'$. The operators $\mathcal{K}_{++}$, $\mathcal{K}_{+-}$ are bounded in $W_2^{3/2}(\Gamma)$, $\mathcal{K}_{-+} = \mathcal{K}^{+}_{+-}$ for real L_0- regular λ and $\mathcal{K}_{--}$ acts from $E_- \subset W_2^{3/2}(\gamma^{\delta}_{\rm out})$ into $W_2^{1/2}(\gamma^{\delta}_{\rm out})$ so that the product $K_-^{-1}\mathcal{K}$ is a bounded operator which can be represented based on the regularized spectral series for the DN-map, as in [30]. Then the expression (5.4) can be written as

$$\mathcal{DN}^F = \mathcal{DN}^{\Delta}_{++} - \mathcal{K}_{++} + \left[\mathcal{DN}^{\Delta}_{+-}\mathcal{K}_{+-}\right] \frac{I}{\mathcal{D}_-} \left[\mathcal{DN}^{\Delta}_{-+} + \mathcal{K}_{-+}\right], \tag{5.16}$$

where the denominator is represented as

$$\mathcal{D}_- = \mathcal{DN}^{\Delta}_{--} + \mathcal{K}_{--} + K_-.$$

Due to special shrinking the positive operator $K_- = |K_-|$ can be estimated from below by the distance $\rho_-(\lambda) = \lambda_{\min} - \lambda$:

$$\langle K_- u,\, u\rangle \geq \rho_- \parallel u \parallel^2_{L_2(\Gamma)} .$$

On the small interval Δ near the Fermi level $\Lambda = 2^{-1}[\lambda_{\min} + \lambda_{\max}]$ this estimate reduces to

$$\langle K_- u,\, u\rangle \geq \frac{\lambda^1_{\min} - \lambda^1_{\max}}{2\delta^2} \parallel u \parallel^2_{L_2(\Gamma)} . \tag{5.17}$$

Definition 5.6. Consider the sum of leading terms in the denominator $\mathcal{D}$ on Δ

$$\mathcal{DN}^{\Delta}_{--} + K_- := \mathcal{D}_0.$$

The pair (μ, e_μ) is called the vector zero of $\mathcal{D}_0$, with root vector e_μ, if

$$\mathcal{D}_0(\mu) e_\mu = 0.$$

The vector zeros of $\mathcal{D}_0$ in a complex neighborhood of Δ are situated on the real axis and can be found from the finite-dimensional equation in E_-:

$$\left[I + K_-^{-1}\mathcal{D}_0\right] e_\mu = 0,$$

of from the corresponding scalar equation

$$\det\left[I + K_-^{-1}\mathcal{D}_0\right](\mu) = 0,$$

see below the calculation in case of a single resonance eigenvalue λ_0, (5.8). For small δ, a vector zero μ_0 of $\mathcal{D}_0$ is localized, due to the operator-valued Rouche theorem, [37], near the resonance eigenvalue λ^δ_0 and the corresponding root vector is close to the corresponding entrance vectors ϕ.

Definition 5.7. We say, that the network is thin on Δ in closed channels, if the sum of leading terms in the denominator $\mathcal{D}_-$

$$\mathcal{DN}^{\Delta}_{--} + K_- = \mathcal{D}_0 \tag{5.18}$$

dominates the remainder

$$\parallel [\mathcal{D}_0]^{-1} \mathcal{K}_{--} \parallel < I$$

on a circle Σ_0 centered at the real zero μ_0 of $\mathcal{D}_0$ in a complex neighborhood of Δ.

If the network is thin on Δ in closed channels, then the disc D_0, $\partial D_0 = \Sigma_0$ contains a simple real vector zero of the denominator $\mathcal{D}$, $\mathcal{D}_-(\mu_0)e_{\mu_0} = 0$, and the corresponding root-vector e_{μ_0} lies in an appropriate neighborhood of the corresponding root vector e_{μ_0} of $\mathcal{D}^0$ (see [37]). In particular $e_{\mu_0} \to \lambda^\delta_0$ and $\mu_0 \to \lambda^\delta_0$ when the network shrinks, $\delta \to 0$.

Theorem 5.8. *If the network is thin on the Fermi-level* Λ *in closed channels, then the pole of the DN-map* $\mathcal{DN}$ *of the operator* L^D *in* $L_2(\Omega^\delta_{\rm int})$ *at the simple resonance eigenvalue* λ^δ_0 *of* L^D *in the first term in the formula* (5.3) *for DN-map of the intermediate Hamiltonian*

$$\mathcal{DN}^F = \mathcal{DN}_{++} - \mathcal{DN}_{+-}\frac{I}{\mathcal{DN}_{--} + \frac{1}{\mu^{\parallel}}K_-}\mathcal{DN}_{-+}$$

is compensated by the corresponding pole of the second addendum and disappears as singularity of the whole function $\mathcal{DN}^\Lambda$, *so that the whole expression* (5.16) *is regular at the point* λ^δ_0. *Generically, a new pole appears as a closest to* λ_0 *zero eigenvalue of the denominator* $\mathcal{D}_0$.

Proof. If the network is thin on Δ in closed channels, then the operator $\mathcal{D}_0$ is invertible: $[\mathcal{D}_0]^{-1} = K_-^{-1/2}\left(I + K_-^{-1/2}\mathcal{K}_{--}K_-^{-1/2}\right)^{-1}K_-^{-1/2}$. Then the middle term of the above product (5.16) can be found as a solution of the equation

$$\left[\frac{\phi_0^-\rangle\langle\phi_0^-}{\lambda-\lambda_0} + \mathcal{K}_{--} + K_-\right]v = f,$$

with $\phi_0^- = P_-\phi_0\big|_\Gamma$, $v = \mathcal{D}_0^{-1}\, f - \frac{1}{\mathbf{D}}\ \mathcal{D}_0^{-1}\,\phi_0^-\rangle\ \langle\phi_0^-,\mathcal{D}_0^{-1}\ f\rangle$, where $\mathbf{D} = (\lambda-\lambda_0) + \langle\phi_0^-,\mathcal{D}_0^{-1}\ \ \phi_0^-\rangle$. Vector-zeroes of the function

$$\left[\frac{\phi_0^-\rangle\langle\phi_0^-}{\lambda-\lambda_0} + \mathcal{K}_{--} + K_-\right] := \mathcal{D}_-(\lambda)$$

coincide with singularities of the middle factor of the second term in the above formula (5.3) for $\mathcal{DN}^F$.

Make sure that substitution of that expression into (5.16) results in mutual compensation of all polar terms containing the factors $(\lambda-\lambda_0)^{-1}$, so that the sum of them vanishes, and, generically, we obtain an expression regular at λ_0. Indeed, taking into account only the terms in (5.16) containing the singularities, the powers of $(\lambda-\lambda_0)^{-1}$ are:

$$\begin{aligned}\frac{\phi_0^+\rangle\langle\phi_0^+}{\lambda-\lambda_0} &- \frac{\phi_0^+\rangle\langle\phi_0^-}{\lambda-\lambda_0}\left[\mathcal{D}_0^{-1} * - \frac{1}{\mathbf{D}}\ \mathcal{D}_0^{-1}\,\phi_0^-\rangle\ \langle\ \mathcal{D}_0^{-1}\phi_0^-,\ *\rangle\right]\left[\frac{\phi_0^-\rangle\langle\phi_0^+}{\lambda-\lambda_0}\right]\\ &- \frac{\phi_0^+\rangle\langle\phi_0^-}{\lambda-\lambda_0}\left[\mathcal{D}_0^{-1} * - \frac{1}{\mathbf{D}}\ \mathcal{D}_0^{-1}\,\phi_0^-\rangle\ \langle\mathcal{D}_0^{-1}\phi_0^-,\ *\rangle\right]\mathcal{K}_{-+}\\ &- \mathcal{K}_{+-}\left[\mathcal{D}_0^{-1} * - \frac{1}{\mathbf{D}}\ \mathcal{D}_0^{-1}\,\phi_0^-\rangle\ \langle\mathcal{D}_0^{-1}\phi_0^-,\ *\rangle\right]\left[\frac{\phi_0^-\rangle\langle\phi_0^+}{\lambda-\lambda_0^0}\right]\\ &+ \frac{\mathcal{K}_{+-}\mathcal{D}_0^{-1}\phi^-\rangle\ \langle\mathcal{K}_{+-}\mathcal{D}_0^{-1}\phi^-}{\mathbf{D}}.\end{aligned} \tag{5.19}$$

The sum of all terms containing $(\lambda-\lambda_0)^{-2}$ can be reduced to:

$$\frac{\phi_0^+\rangle\ \langle\phi_0^+}{(\lambda-\lambda_0)^2}\left[(\lambda-\lambda_0) - \frac{\langle\phi_0^-,\mathcal{D}_0^{-1}\phi_0^-}{I + \frac{\langle\phi_0^-,\mathcal{D}_0^{-1}\phi_0^-}{\mathbf{D}}})\right] = \frac{\phi_0^+\rangle\ \langle\phi_0^+}{\mathbf{D}}.$$

The terms containing $(\lambda - \lambda_0)^{-1}$ and $\mathcal{K}_{+-}$, $\mathcal{K}_{-+}$ as well as the square bracket

$$\left[\mathcal{D}_0^{-1} * - \frac{1}{\mathbf{D}}\ \mathcal{D}_0^{-1}\ \phi_0^-\rangle\ \langle\ \mathcal{D}_0^{-1}\phi_0^-,\ *\rangle\right]$$

can be transformed for $\mathcal{K}_{+-}$ as

$$-\frac{\mathcal{K}_{+-}\mathcal{D}_0^{-1}\phi_0^-\rangle\ \langle\phi_0^-}{(\lambda - \lambda_0)} + \frac{\mathcal{K}_{+-}\ \mathcal{D}_0^{-1}\phi_0^-\rangle\ \langle\ \phi_0^-, \mathcal{D}_0^{-1}\ \phi_0^-\rangle\ \langle\phi_0^+}{\mathbf{D}}(\lambda - \lambda_0) =$$

$$-\ K_{+-}\mathcal{D}_0^{-1}\ \phi_0^-\ \rangle\mathbf{D}^{-1}\ \langle\ \phi_0^+$$

and, similarly, for the sum of terms containing $\mathcal{K}_{-+} = \mathcal{K}_{+-}^+$ we have:

$$-\ \phi_0^+\rangle\mathbf{D}^{-1}\ \langle K_{+-}\mathcal{D}_0^{-1}\ \phi_0^-.$$

Collecting the transformed terms we obtain for thin network in closed channels at λ_0, we get

$$\mathcal{D}N^\Lambda = \frac{\phi_0^+ - \mathcal{K}_{+-}\mathcal{D}_0^{-1}\ {\phi_0}^-\rangle\ \langle{\phi_0}^+ - \mathcal{K}_{+-}\mathcal{D}_0^{-1}\ \phi_0^-}{\mathbf{D}} + \cdots, \tag{5.20}$$

where the dots represent the terms defining regular summands of $\mathcal{DN}^\Lambda$ in a small neighborhood of the resonance eigenvalue. Comparing the above expression (5.20) with the spectral representation of $\mathcal{DN}^F$, we conclude that

$$\frac{\phi_0^+ - \mathcal{K}_{+-}\mathcal{D}_0^{-1}\ {\phi_0}^-\rangle\ \langle{\phi_0}^+ - \mathcal{K}_{+-}\mathcal{D}_0^{-1}\ \phi_0^-}{\mathbf{D}} = \mathcal{D}N_\Delta^F \tag{5.21}$$

coincides with the polar term of $\mathcal{D}N^F$ at the resonance eigenvalue. Hence the zero of the denominator $\mathbf{D}$ is the resonance eigenvalue of the intermediate Hamiltonian L^F and $\phi_0^+ - \mathcal{K}_{+-}\mathcal{D}_0^{-1}\ {\phi_0}^-$ is the corresponding resonance entrance vector which defines the resonance properties of the scattering matrix. □

Corollary 5.9. *Inserting the resonance expression $\mathcal{DN}_\Delta^F$ for the polar term of $\mathcal{DN}^F$ we obtain a convenient rational approximation for the scattering matrix near the resonance:*

$$S_{\text{approx}}(\lambda) = \frac{iK_+/\mu^{\|} + \mathcal{DN}_\Delta^F}{iK_+/\mu^{\|} - \mathcal{DN}_\Delta^F}. \tag{5.22}$$

Summarizing the formulae (5.14), (5.15), and (5.18)) for the approximate resonance eigenvalue λ_0^δ of L^D, for the corresponding resonance entrance vector ϕ_0, and for leading terms of the denominator $\mathcal{D}_0$, we obtain an approximate expression for $\mathcal{DN}_\Delta^F$ and for the scattering matrix, based on (5.22). The non-diagonal matrix elements of this formula define the transmission coefficients, similarly to the corresponding formula in [26] and the corresponding formulae for the solvable models in [19, 21].

Remark 5.10. In fact, based on (5.13) even better approximation of the scattering matrix can be obtained. One can see that on the first step of the approximation procedure we obtain the pole of $\mathcal{D}N^F$ at the simple zero of the denominator bfD with the same residue ${\phi_0}^+\rangle\ \langle{\phi_0}^+$ as in $\mathcal{D}N$, in full agreement with physical folklore.

For thin network we obtain: $[\mathcal{D}_0]^{-1} = K_-^{-1} - K_-^{-1}\mathcal{K}_- K_-^{-1} + \cdots$. Substituting this expression into the denominator $\mathbf{D}$ and into the resonance entrance vector $\phi_0^+ - \mathcal{K}_{+-}k^{-1}\,\phi_0{}^-$ we can obtain an approximate expressions for the resonance eigenvalue of the intermediate Hamiltonian and for the leading term $\mathcal{DN}_\Delta^F$ of the DN-map $\mathcal{DN}^F$ of the intermediate Hamiltonian. This opens a way to calculation of the spectral parameters of the intermediate Hamiltonian based on spectral data of L^D. These data can be obtained with use of standard software. We postpone to forthcoming papers the derivation of the corresponding approximate formulae for the scattering matrix and calculation of resonances based on [37].

6. Appendix: the intermediate Hamiltonian

The role of the single-electron Hamiltonian on the quantum network Ω is played by the Schrödinger operator

$$2m_0\,\hbar^{-2}\mathcal{L}_R u = -\,\triangle_\mu\, u + V(x)u + h_r u \tag{6.1}$$

with

$$h_r = \begin{cases} 2m_0\,\hbar^{-2}H_R & \text{if } x,y\in\Omega_{\text{int}},\\ 0 & \text{if } x,y\in\Omega_{\text{out}} = \cup_m\omega_m, \end{cases}$$

with appropriate boundary conditions (3.4) on Γ and Dirichlet boundary conditions on $\partial\Omega$. The kinetic term $-\triangle_\mu$ containing the tensor μ of scaled effective masses is

$$-\triangle_\mu = \begin{cases} -(\mu^*)^{-1}\triangle\ , & \text{if } x,y\in\Omega_{\text{int}},\\ -\frac{1}{\mu^{\|}}\frac{\partial^2}{\partial x^2} - \frac{1}{\mu^{\perp}}\frac{\partial^2}{\partial y^2}, & \text{if } x,y\in\omega^m, \end{cases}$$

where x,y are the local coordinates. We impose Meixner conditions at the inner corners of Ω_{int} in form $D\mathcal{L}\subset W_2^1(\Omega)$, Dirichlet boundary conditions on $\partial\Omega$ and appropriate matching conditions (3.4) on Γ. Formally full Hamiltonian on the network is obtained as the Friedrichs extension of the symmetric operator defined by the same differential expression and the matching condition (3.4) on smooth functions vanishing near the boundary $\partial\Omega$.

The intermediate Hamiltonian is defined by operator splitting procedure, see [32] depending on the scaled Fermi-level Λ_F. The non-perturbed Schrödinger operator via separation of variables is reduced to the orthogonal sum $L_{\text{out}} = \oplus\sum_{s,n} l_{s,n}$ of one-dimensional Schrödinger operators in $\mathcal{H}_{m,n} = L_2(0,\infty)\times e_{s,n}$:

$$l_{s,n} = -\frac{1}{\mu^{\|}}\frac{\partial^2}{\partial x^2} - \frac{n^2\,\pi^2}{\delta^2\mu^{\perp}} I_{s,n},\quad s = 1,2,3.$$

Here $I_{s,n}$ is the unit operator in the "channel space" $\mathcal{H}_{s,n}$, $e_{s,n} = \sin\frac{n\,\pi\,y}{\delta}$ is the cross-section eigenfunction on the wire ω_s, with the eigenvalue $\lambda_{s,n} = \frac{\pi^2\,n^2}{2\delta^2\mu^{\perp}}$.

Formal solutions of the equation $l_{s,n}\Phi = \lambda\Phi$ are

$$\Phi_{s,n}(x) = \sinh\sqrt{\lambda_{s,n} - \lambda}\,x, \quad \text{if } \lambda < \lambda_{s,n}, \text{ and}$$
$$\Phi_{s,n}(x) = \sin\sqrt{\lambda - \lambda_{s,n}}\,x, \quad \text{if } \lambda > \lambda_{s,n}.$$

The operator L_{out} has absolutely-continuous spectrum consisting of a countable system of branches $\sigma_{s,n} := [\lambda_{s,n}, \infty)$ with thresholds $\lambda_{s,n}$, which correspond to the parts $l_{s,n}$ in the channels $\mathcal{H}_{s,n}$; see [36]. For given Fermi level $\Lambda_F \neq \lambda_{s,n}$, we call the channels with $\lambda_{s,n} < \Lambda_F$ *open channels*, and ones with $\lambda_{m,n} > \Lambda_F$ *closed channels.* The corresponding thresholds $\lambda_{s,n}$ are called *upper* and *lower* thresholds, respectively. Denote by λ^F_{min} the minimal upper threshold in semi-infinite wires:

$$\lambda^F_{\text{min}} = \min_{\frac{s^2\pi^2}{\mu^\perp\delta^2} > \Lambda^F} \left\{\frac{s^2\pi^2}{\mu^\perp\delta^2}\right\} := \min_{\text{closed}} \left\{\frac{s^2\pi^2}{\mu^\perp\delta^2}\right\},$$

and by λ^F_{max} the maximal lower threshold (of open channels):

$$\lambda^F_{max} = \max_{\frac{n^2\pi^2}{\mu^\perp\delta^2} < \Lambda^F} \left\{\frac{n^2\pi^2}{\mu^\perp\delta^2}\right\} := \max_{\text{open}} \left\{\frac{s^2\pi^2}{\mu^\perp\delta^2}\right\},$$

The spectral band $\left[\lambda^F_{\text{max}}, \lambda^F_{\text{min}}\right] := \Delta_F$ contains the scaled Fermi level Λ^F and plays a role of the *conductivity band.* For $\lambda \in \Delta^F$ the exponential solutions of the Schrödinger equation in the wires are either

- exponentially growing/decreasing in "closed channels" $\frac{n^2\pi^2}{\mu^\perp\delta^2} > \Lambda_F$,

$$(\delta/2)^{-1/2} \sin\left(\frac{n\,\pi\,y}{\delta_m}\right) e^{\pm\sqrt{\mu^\parallel}\sqrt{\left[\frac{n^2\pi^2}{\mu^\perp\delta^2} - \lambda\right]}} := e_{s,n}(y)\, e^{\pm k_-(\lambda,n)x} = e^{\pm K_- x}\, e_{s,n},$$

  with a positive diagonal matrix $K_- = \lceil k^n_- \rfloor$ acting in the *entrance subspace* of closed channels $E_- = \bigvee_{\text{closed}} \sin\frac{n\,\pi\,y}{\delta}$, or
- just oscillating in "open channels" $\frac{s^2\pi^2}{2\mu^\perp\delta^2} < \Lambda^F$,

$$(\delta/2)^{-1/2} \sin\left(\frac{n\,\pi\,y}{\delta}\right) e^{\pm i\sqrt{\mu^\parallel}\sqrt{\lambda - \left[\frac{s^2\pi^2}{\mu^\perp\delta^2}\right]}} := e_{s,n}(y)\, e^{\pm ik_+(\lambda,n)x} = e^{\pm i\,K_+ x}\, e_{s,n},$$

  with a positive diagonal matrix $K_+ = \lceil k_+(\lambda, n)\rfloor$ acting in the *entrance subspace* of the open channels, $E_+ = \bigvee_{\text{open}} \sin\frac{n\,\pi\,y}{\delta_m} = L_2(\Gamma) \ominus E_-$, $\dim E_+ < \infty$, $\dim E_- = \infty$.

Elements from the domain $D(\mathcal{L})$ of the Schrödinger operator $\mathcal{L}$ on the whole network Ω belong locally (outside a small neighborhood of inner corners) to the appropriate Sobolev class, $D(\mathcal{L}) \subset W^2_{2,\text{loc}}(\Omega_t)$, see [31, 35].

For given scaled Fermi level $\Lambda^F > 0$ we define in $L_2(\Omega)$ the split Hamiltonian via operator splitting, [32], following [26], based on the same differential expression as original Schrödinger operator $\mathcal{L}$ but *choose the domain depending on Fermi level* F. Denote by $P_\pm$ the orthogonal projections in $L_2(\Gamma)$ onto $E_\pm$, respectively. Denote by u_{out}, u_{int} vector-function $\mathbf{u} = \{\oplus\sum_m \oplus u_m, u_{\text{in}}\}$, obtained via restriction of the function u defined on the whole network, onto $\Omega_{\rm out}$ and $\Omega_{\rm int}$, respectively. The domain of the split operator $\mathcal{L}_F$ is described by the boundary condition:

$$P_+ u_{\rm int}\Big|_\Gamma = P_+ u_{\rm out}\Big|_\Gamma = 0,\ \ P_- \left[u_{\rm int} - u_{\rm out}\right]\Big|_\Gamma = 0,$$

$$P_- \left[-\frac{1}{\mu^*}\frac{\partial}{\partial n_\xi} + \frac{i\alpha\, m_0}{2\hbar}\left[\sigma,\, n\right]_y + \frac{1}{\mu^{\|}}\frac{\partial u_{\rm out}}{\partial n}\right]\Bigg|_\Gamma = 0. \qquad (6.2)$$

The split operator is reduced by the orthogonal decomposition

$$\mathcal{H}_+ \oplus \left[L_2(\Omega) \ominus \mathcal{H}_+\right].$$

The part l_F of $\mathcal{L}_F$ in open channels coincides with $\oplus\sum_{\rm open} l_{s,n}$, $\mathcal{L}_F = L_F \oplus l_F$. The part l_F of $\mathcal{L}_F$ in open channels coincides with $\oplus\sum_{\rm open} l_{s,n}$ and has pure absolutely continuous spectrum $\sigma(l_F) = \cup_{\rm open}\sigma_{m,n} \supset \Delta_f$. The part L_F of $\mathcal{L}_F$ in $L_2(\Omega)\ominus\mathcal{H}_+$ plays the role of an intermediate Hamiltonian. It is self-adjoint and it's absolutely-continuous spectrum coincides with the union of branches of the absolutely- continuous spectrum of $L_{\rm out}$ in closed channels, $\sigma(L_F) = \cup_{\rm closed}\sigma_{m,n}$. In particular, it does not contain the conductivity band Δ_F. The following statement contains complete description of spectral properties of the operators $\mathcal{L}_R$, L_R:

Theorem 6.1. *Consider the operators L_F, l_F, and $\mathcal{L}_F = L_F \oplus l_F$, defined by the differential expression* (2.3)*, the above boundary conditions* (3.4) *and Meixner condition at the inner corners on the boundary. The domain of the operator l_F consists of all locally W_2^2-smooth functions from the direct sum of all open semi-infinite channels $\mathcal{H}_+$ in the semi-infinite wires. The domain of the operator L_F consists of W_2^2-smooth functions on the well and the joining wires which belong to $\mathcal{H}_- = L_2(\Omega)\ominus\mathcal{H}_+$ and satisfy the boundary conditions* (3.4) *on* Γ. *Both operators L_F, l_F are self-adjoint. The absolutely-continuous spectra $\sigma_a(l_F)$, $\sigma_a(L_F)$ of l_F, L_F coincide with the union of all lower and all upper branches in semi-infinite wires, respectively:*

$$\sigma_a(l_F) = \bigcup_{\left\{\frac{n^2\pi^2}{\mu^\perp\delta^2}<\Lambda\right\}} \left[\frac{n^2\,\pi^2}{\mu^\perp\delta^2},\, \infty\right), \quad \sigma_a(L_F) = \bigcup_{\left\{\frac{n^2\pi^2}{\mu^\perp\delta^2}>\Lambda\right\}} \left[\frac{n^2\,\pi^2}{\mu^\perp\delta^2},\, \infty\right).$$

The absolutely-continuous spectrum $\sigma_a(\mathcal{L})$ of the operator $\mathcal{L}$ coincides with the absolutely-continuous spectrum of the split operator $\mathcal{L}_F = L_F \oplus l_F$:

$$\sigma_a(\mathcal{L}) = \sigma_a(\mathcal{L}_F) = \sigma_a(l_F) \cup \sigma_a(L_F)$$

Besides absolutely continuous spectrum, the operators $\mathcal{L}$ and L_F may have a finite number of eigenvalues below the threshold of the absolutely-continuous spectrum and a countable sequence of embedded eigenvalues accumulating at infinity. The singular continuous spectrum of both $\mathcal{L}$, $\mathcal{L}_F$ is absent.

The original Hamiltonian $\mathcal{L}$ on the whole network is obtained from the split operator $\mathcal{L}_F = L_F \oplus l_F$ via a finite-dimensional perturbation, replacing the first of the boundary conditions by the corresponding matching boundary condition (3.4).

Proof. for the Schrödinger operator without Rashba Hamiltonian may be found in [34, 33]. In presence of Rashba Hamiltonian the proof follows the pattern of [34, 33]. □

7. Conclusion

Based on above approximate formula for the scattering matrix one can optimize the shape of the well to enhance the selectivity of the spin filter. We anticipate an application of our formulae for the solution of the second problem formulated in the introduction: withdrawal from the scattering system of electrons with the certain value of the spin. We guess that the solution of the problem may be achieved via using of specially shaped Quantum Networks constructed on the surface of a narrow-gap semiconductor.

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Quantum graph in a magnetic field and resonance states completeness

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To the memory of Boris Pavlov

Abstract. Quantum graph with the Landau operator (Schrödinger operator with a magnetic field) at the edges is considered. The Kirchhoff condition is assumed at the internal vertices. We derive conditions for the graph structure ensuring the completeness of the resonance states on finite subgraphs obtained by cutting all infinite leads of the initial graph. Due to the use of a functional model, the problem reduces to factorization of the characteristic matrix-function. The result is compared with the corresponding completeness theorem for the Schrödinger quantum graph.

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1. Introduction

The oldest result concerning to resonances was obtained for the Helmholtz resonator by Rayleigh a century ago. There are many works describing resonances for various physical problems (see, e.g., [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14, 15]). The completeness problem for the resonance states began to discuss essentially later, in 70th [16], but answers were found for a few particular cases only (see, e.g., [17, 18]).

There is an interesting relation between this problem and the Sz.-Nagy functional model [19, 20, 21]. Starting with work [22], it is known that the scattering matrix is the same as the characteristic function from the functional model. Moreover, root vectors in the functional model correspond to resonance states in scattering theory. The problem of completeness of the system of root vectors is related to the factorization problem for the characteristic function. It allows one to

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study the completeness using factorization. Particularly, for the finite-dimensional case, this approach gives one an effective completeness criterion [20].

Recently, the completeness results were obtained for a few problems on quantum graphs, namely, for the Schrödinger and Dirac operators on some graphs and hybrid manifolds [24, 25, 26, 27]. In the present paper we consider the Schrödinger operator with a magnetic field. The Kirchhoff condition is assumed at the internal vertices of the graph. We obtain the condition for the graph structure which ensures the completeness of the resonance states on the subgraph obtained by cutting infinite leads. The proof is based on results of [28, 29, 30].

2. Preliminaries

2.1. Quantum graph model

Let us first describe the structure of the quantum graph Γ under consideration. We start with a finite compact metric graph Γ_0 (with the set of edges E^{int}, named as internal edges), choose some subset of vertices V^{ext}, to be called external vertices, and attach one or more copies of semi-axis $[0;\infty)$, to be called leads (E^{ext}), to each external vertex. We identify the point 0 in a lead with the relevant external vertex. The thus extended graph is the graph Γ in question. Let V be the set of all vertices of Γ. Correspondingly, $V^{\text{int}} = V \setminus V^{\text{ext}}$; the elements of V^{int} will be called internal vertices. For convenience, we assume that Γ has no edge starts and ends at the same vertex. If it is not so, one can introduce additional vertices, which do not change the situation, really.

Definition 2.1. A vertex is named “external” if it has semi-infinite lead attached and ”internal” in the opposite case.

Definition 2.2. An external vertex is named “balanced” if for this vertex the numbers of attached leads equals to the number of attached edges. is not balanced, we call it unbalanced.

As for the differential operator on the edges and leads, we consider two cases: one-dimensional free Schrödinger operator (i.e., the second derivative: $H = -\frac{d^2}{dx^2}$) and the Landau operator (one-dimensional Schrödinger operator with a magnetic field: $H = -(\frac{d}{dx} + iA_j$, A_j is the tangent component of the vector potential corresponding to the magnetic field for edge A_j; without loss of generality, we may assume that it is zero on external leads because on an edge which is not a part of a loop we can easily remove the vector potential by a gauge transformation). We will assume that the metric graph belongs to a plane embedded in $\mathbb{R}^3$ and has no “false” edge intersections, i.e., “intersections without vertices”. The magnetic field is orthogonal to this plane. This assumption is not necessary but simplifies the consideration. The domain of H consists of continuous functions on Γ, belonging to W_2^2 on each lead and edge satisfying the boundary conditions at boundary vertices (we assume the Dirichlet condition), coupling conditions at other vertices (we assume the Kirchhoff condition):

$$\sum_{e,v\in e}(-1)^{\kappa(e(v))}\frac{\partial\psi}{\partial x}=0, \tag{2.1}$$

where $\kappa(e(v))=0$ for outgoing edge/lead e and $\kappa(e(v))=1$ for incoming edge e. Note that all leads were chosen as outgoing.

The standard definition of resonance is as follows

Definition 2.3. We will say that $k^2\in\mathbb{C}, k\neq 0$, is a resonance of H (or, by a slight abuse of terminology, a resonance of Γ) if there exists a resonance eigenfunction (resonance state) $f, f\in L^2_{\text{loc}}\Gamma$, which satisfies the differential equation

$$Hf(x)=k^2f(x),\quad x\in\Gamma,$$

on each edge and lead of Γ, is continuous on Γ, satisfies the boundary conditions at boundary vertices, coupling conditions at other vertices, and the radiation condition $f(x)=f(0)e^{ikx}$ on each lead.

We denote the set of resonances as Λ. One can give another, equivalent, definition of resonances in the framework of the Lax–Phillips scattering theory (see below).

We define the resonance counting function by

$$N(R)=\sharp\{k:k\in\Lambda,|k|\leq R\},\quad R>0$$

(each resonance is counted with its algebraic multiplicity). Note that the set Λ of resonances is invariant under the symmetry $k\to-\overline{k}$, so this method of counting yields, roughly speaking, twice as many resonances as one would obtain if one imposed an additional condition $\Re(k)\geq 0$. In particular, in the absence of leads, $N(R)$ equals twice the number of eigenvalues $\lambda\neq 0$ of H (counting multiplicities) with $\lambda\leq R^2$.

There are works concerning to asymptotics of resonances in the complex plane [28, 30, 29]. If there are no leads then H has the pure point spectrum, there are no resonances, but we can say that resonances are identified with eigenvalues of H, and it is known that for these eigenvalues, one has Weyl's law:

$$N(R)=\frac{2}{\pi}\text{vol}(\Gamma_0)R+o(R),\quad \text{as } R\to\infty, \tag{2.2}$$

where $\text{vol}(\Gamma_0)$ is the sum of the lengths of the edges of Γ_0 which plays the role of volume in general Weyl formula. We say that Γ (i.e., the corresponding graph with leads) is a Weyl graph, if the asymptotics (2.2) takes place for resonances of Γ.

The following theorem was proved in [28].

Theorem 2.4. *One has*

$$N(R)=\frac{2}{\pi}WR+O(1),\quad \textit{as } R\to\infty, \tag{2.3}$$

where the coefficient W satisfies $0\leq W\leq\text{vol}(\Gamma_0)$. One has $W=\text{vol}(\Gamma_0)$ if and only if every external vertex of Γ is unbalanced.

2.2. Scattering, functional model and completeness criterion

For our purposes, it is convenient to consider the scattering in the framework of the Lax–Phillips approach [32]. Consider the Cauchy problem for the time-dependent Schrödinger equation with a magnetic field on the graph Γ:

$$\begin{cases} i\hbar u_t' = Hu, \\ u(x,0) = u^0(x), \ x \in \Gamma. \end{cases} \tag{2.4}$$

Let $U(t)$ be unitary operator in the state space $\mathcal{E}$ (of initial data) giving the solution of the Cauchy problem (2.4): $u(x,t) = U(t)u^0(x)$; $U(t)|_{t\in\mathbb{R}}$ forms a continuous, one parameter, evolution unitary group of operators in $\mathcal{E}$. There are two orthogonal subspaces D_- and D_+ in $\mathcal{E}$, correspondingly called the incoming and outgoing subspaces.

Definition 2.5. The outgoing (incoming) subspace D_+, D_- is a subspace of $\mathcal{E}$ having the following properties:

(a) $U(t)D_+ \subset D_+$ for $t > 0$; $U(t)D_- \subset D_-$ for $t < 0$;

(b) $\bigcap_{t>0} U(t)D_+ = \{0\}$; $\bigcap_{t<0} U(t)D_- = \{0\}$;

(c) $\overline{\bigcup_{t<0} U(t)D_+} = \mathcal{E}$, $\overline{\bigcup_{t>0} U(t)D_-} = \mathcal{E}$.

For the graph Γ, the subspace D_+ contains functions vanishing at Γ_0 (e.g., on all edges of finite length) and satisfying the radiation condition on all leads.

Let $P_\pm$ be the orthogonal projection of $\mathcal{E}$ onto the orthogonal complement of $D_\pm$. Consider the semigroup $\{Z(t)\}|_{t\geq 0}$ of operators on $\mathcal{E}$ defined by

$$Z(t) = P_+U(t)P_-, \quad t \geq 0.$$

Lax and Phillips proved the following theorem [32].

Theorem 2.6. *The operators $\{Z(t)\}|_{t\geq 0}$ annihilate D_+ and D_-, map the orthogonal complement subspace $K = \mathcal{E} \ominus (D_- \oplus D_+)$ into itself and form a strongly continuous semigroup (i.e., $Z(t_1)Z(t_2) = Z(t_1 + t_2)$ for $t_1, t_2 \geq 0$) of contraction operators on K. Furthermore, we have $s\text{-}\lim_{t\to\infty} Z(t) = 0$. The space $\mathcal{E}$ can be represented isometrically as the Hilbert space of functions $L_2(\mathbb{R}, N)$ for some auxiliary Hilbert space N in such a way that $U(t)$ goes to translation to the right by t units and D_+ is mapped onto $L_2(\mathbb{R}_+, N)$. This representation is unique up to an isomorphism of N.*

Definition 2.7. Let B be the generator of the semigroup $Z(t) : Z(t) = \exp i\mathsf{B}t, t > 0$. The eigenvalues of B are called resonances and the corresponding eigenvectors are the resonance states.

Such a representation is called an outgoing translation representation. Analogously, one can obtain an incoming translation representation, i.e., if D_- is an incoming subspace with respect to the group $\{U(t)\}_{t\in\mathbb{R}}$ then there is a representation in which $\mathcal{E}$ is mapped isometrically onto $L_2(\mathbb{R}, N)$, $U(t)$ goes to translation to the right by t units and D_- is mapped onto $L_2(\mathbb{R}_-, N)$.

The Lax–Phillips scattering operator $\tilde{S}$ is defined as follows (it was proved that this definition is equivalent to the standard one). Suppose $W_+ : \mathcal{E} \to L_2(\mathbb{R}, N)$ and $W_- : \mathcal{E} \to L_2(\mathbb{R}, N)$ are the mappings of $\mathcal{E}$ onto the outgoing and incoming translation representations, respectively. The map $\tilde{S} : L_2(\mathbb{R}, N) \to L_2(\mathbb{R}, N)$ is defined by the formula

$$\tilde{S} = W_+(W_-)^{-1}.$$

For most purposes it is more convenient to work with the incoming spectral representation and the outgoing spectral representation which are the Fourier transforms F, correspondingly, of the incoming and the outgoing translation representations. Respectively, $D_{-(+)}$ transforms to $H^2_{+(-)}(\mathbb{R}, N)$, i.e., to the space of boundary values on $\mathbb{R}$ of functions in the Hardy space $H^2(\mathbb{C}^{+(-)}, N)$ of vector-valued functions (with values in N) defined in the upper (lower) half-plane $\mathbb{C}^{+(-)}$. Accordingly, the scattering operator $\tilde{S}$ in the spectral representation is given by the following formula

$$S = F\tilde{S}F^{-1}.$$

The operator S acts as the operator of multiplication by the operator-valued function $S(\cdot)$ on $\mathbb{R}$. $S(\cdot)$ is called the Lax–Phillips S-matrix. The main properties of S are presented in the following theorem [32].

Theorem 2.8. (a) $S(\cdot)$ *is the boundary value on* $\mathbb{R}$ *of an analytic in* $\mathbb{C}^+$ *operator-valued function,*

(b) $\|S(z)\| \le 1$ *for every* $z \in \mathbb{C}^+$*,*

(c) $S(E)$*,* $E \in \mathbb{R}$*, is, pointwise, a unitary operator on* N*.*

The analytic continuation of $S(\cdot)$ from the upper to the lower half-plane is obtained by a conventional procedure:

$$S(z) = (S^*(\overline{z}))^{-1}, \quad \Im z < 0.$$

Finally, $S(\cdot)$ is a meromorphic operator-valued function on the whole complex plane (we do not change the notation for the operator-function). There is a relation between the eigenvalues of B and the poles of the S-matrix. It is described in the following theorem from [32].

Theorem 2.9. *If* $\Im k < 0$*, then* k *belongs to the point spectrum of* B *if and only if* $S^*(\overline{k})$ *has a non-trivial null space.*

Remark 2.10. The theorem shows that a pole of the Lax–Phillips S-matrix at a point k in the lower half-plane is associated with an eigenvalue k of the generator of the Lax–Phillips semigroup. In other words, resonance poles of the Lax–Phillips S-matrix correspond to eigenvalues of the Lax–Phillips semigroup with well defined eigenvectors belonging to the subspace $K = \mathcal{E} \ominus (D_- \oplus D_+)$, which is called the resonance subspace.

Theorem 2.11. *There is a pair of isometric maps* $T_\pm : \mathcal{E} \to L_2(\mathbb{R}, N)$ (*the outgoing and incoming spectral representations*) *having the following properties:*

$$T_\pm U(t) = e^{ikt} T_\pm, \quad T_\pm D_\pm = H^2_\pm(N), \quad T_- D_+ = SH^2_+(N),$$

where $H^2_\pm(N)$ *is the Hardy space of the upper* (*lower*) *half-plane, the matrix-function* S *is an inner function in* $\mathbb{C}_+$*, and*

$$K_- = T_- K = H^2_+ \ominus SH^2_+, \quad T_- Z(t)|_K = P_{K_-} e^{ikt} T_-|_{K_-}.$$

There is an interesting relation between the completeness of the system of resonance states (i.e., root vectors of B) and the factorization of the scattering matrix. Namely, as an inner function, S can be represented in the form $S = \Pi\Theta$, where Π is a Blaschke–Potapov product (operator-function generalization of scalar Blaschke product [23]) and Θ is a singular inner function [19, 20, 21]. The next theorem shows this relation.

Theorem 2.12 (Completeness criterion [20]**).** *The following statements are equivalent:*

1. *The system of root vectors of the operator* B *is complete;*
2. *The system of root vectors of the operator* B^* *is complete;*
3. S *is a Blaschke–Potapov product.*

There is a simple criterion for the absence of the singular inner factor in the case $\dim N < \infty$ (in the general operator case there is no such simple criterion).

Theorem 2.13 ([20]**).** *Let* $\dim N < \infty$*. The following statements are equivalent:*

1. S *is a Blaschke–Potapov product;*
2. $$\lim_{r\to 1} \int_0^{2\pi} \frac{\mathsf{R}(r)\ln(s(\mathsf{R}(r)e^{it} + i\mathsf{C}(r)))}{(\mathsf{R}(r)e^{it} + i\mathsf{C}(r) + i)^2} dt = 0, \tag{2.5}$$

   where

   $$s(k) = |\det S(k)|, \quad \mathsf{C}(r) = \frac{1+r^2}{1-r^2}, \quad \mathsf{R}(r) = \frac{2r}{1-r^2}. \tag{2.6}$$

Remark 2.14. The corresponding theorem in [20] was proved for unit disk. We reformulate it for the upper half-plane. It should be noted that $\mathsf{R} \to \infty$ corresponds to $r \to 1$.

Our main theorem is as follows.

Theorem 2.15 (Main theorem). *The system of resonance states of operator* H *is complete on* $L^2(\Gamma_0)$ *if and only if every external vertex of* Γ *is unbalanced.*

3. Proof of the main theorem

To prove the completeness or incompleteness of resonance states, we follow the way analogous to that used in [28] for investigation of resonance asymptotics. Namely, the proof splits into two cases corresponding to presence or absence of balanced vertices.

3.1. Relation between magnetic and non-magnetic cases

It is well-known (see, e.g., [30, 33]) that using the local gauge transformation, one can get rid of the explicit dependence of the magnetic field and arrive thus at the free Hamiltonian with the transformed coupling conditions. Let us describe the transformation. Let the graph be embedded in $\mathbb{R}^3$. Consider an edge e which is parameterized by a natural way $r(x) = (r_1(x), r_2(x), r_3(x))$, $r : [0, L_e] \to \mathbb{R}^3$, $|\dot{r}| \equiv 1$ (here dot means the derivative in the parameter x). The magnetic field is introduced using the vector potential $\vec{A} : \mathbb{R}^3 \to \mathbb{R}^3$. The Schrödinger operator with a magnetic field in $\mathbb{R}^3$ has the form

$$H\psi(r) = -\big(\nabla - i\vec{A}\big)^2\psi,$$

where we choose a system of units such that $e = \hbar = 1$, $m = 1/2$. As in the considered case the movement is confined by the curve, the magnetic momentum operator is confined to the tangential direction to the curve e:

$$\dot{r} \cdot \big(\nabla - i\vec{A}\big)f = \dot{r}\,(\nabla f) - i\big(\dot{r}\vec{A}\big)f = \frac{\partial}{\partial x}f(r(x)) - iA_e(x)f(r(x)),$$

where $A_e(x) = \dot{r}(x) \cdot \vec{A}(r(x))$. Correspondingly, at the curve, one has

$$H\psi(x) = -\left(\frac{\partial}{\partial x} - iA_e\right)\psi(x).$$

Let us make a replacement

$$\psi(x) = g(x)\exp\left[i\int\limits_0^x A_e(\tau)d\tau\right].$$

Then,

$$\begin{aligned}\left(\frac{\partial}{\partial x} - A_e i\right)&e^{i\int_0^x A_e(\tau)d\tau}g(x)\\ &= -A_e i\psi(x) + g'(x)e^{i\int_0^x A_e(\tau)d\tau} + g(x)iA_e(x)e^{i\int_0^x A_e(\tau)d\tau}\\ &= e^{i\int_0^x A_e(\tau)d\tau}\frac{\partial}{\partial x}g(x).\end{aligned}$$

Hence,

$$He^{i\int_0^x A_e(\tau)d\tau} = e^{i\int_0^x A_e(\tau)d\tau}\left(-\frac{\partial^2}{\partial x^2}\right).$$

Correspondingly, the Schrödinger equation $H\psi = E\psi$ is equivalent to the following equation:

$$-\frac{\partial^2}{\partial x^2}g = Eg.$$

That is, g satisfies the free Schrödinger equation. As for the boundary conditions, note that the magnetic derivative is more natural from the physical point of view: $\partial = \dfrac{\partial}{\partial x} - ia$. The corresponding Kirchhoff condition has the form:

$$\begin{cases} \psi_e(v) = \psi_{e'}(v) \quad \forall e, e' : v \in e, v \in e'; \\ \sum\limits_{e \sim v} \partial\psi(e(v) = 0. \end{cases}$$

As

$$\begin{aligned} \partial\psi_e(x) &= \partial\left(e^{i\int\limits_0^x A_e(\tau)d\tau} g(x)\right) - A_e i g(x) e^{i\int\limits_0^x A_e(\tau)d\tau} \\ &= g'(x)e^{i\int\limits_0^x A_e(\tau)d\tau} + g(x)iA_e(x)e^{i\int\limits_0^x A_e(\tau)d\tau} - A_e i g(x)e^{i\int\limits_0^x A_e(\tau)d\tau} \\ &= g'(x)e^{i\int\limits_0^x A_e(\tau)d\tau}, \end{aligned}$$

one has

$$\begin{cases} \partial\psi_e(0) = g_e'(0); \\ \partial\psi_e(l) = g_e'(l)e^{i\Phi}; \\ \psi_e(0) = g_e(0); \\ \psi_e(l) = g_e(l)e^{i\Phi}. \end{cases}$$

Thus, the magnetic Kirchhoff conditions for g takes the form

$$\begin{cases} e^{i\Phi_e(v)} g_e(v) = g_{e'}(v)e^{i\Phi_{e'}(v)}; \\ \sum\limits_e g_e'(v)e^{i\Phi_e(v)} = 0, \end{cases}$$

where

$$\Phi_e(v) = \begin{cases} 0, & \text{if } v \text{ is the beginning of edge} e; \\ \int\limits_0^t a_e(\tau)d\tau, & \text{if } v \text{ is the end of edge } e. \end{cases}$$

The described relation ensures close similarity of the completeness proofs for the cases of presence or absence of the magnetic field.

Remark 3.1. In the considered case, this transformation is not necessary because due to absence of a potential, one constructs the explicit solutions at the graph edges. But the transformation can be performed in a general case when a potential is presented.

To construct the scattering matrix for the graph Γ we solve a series of scattering problems each of them corresponds to wave coming from a selected lead. We assume that all leads are straight and orthogonal to the magnetic field. Correspondingly, we can deal with the free Schrödinger operator at these lines. If we consider a wave coming from jth lead the solution on jth lead has the form $e^{-ikx} + s_{jj}e^{ikx}$ and on pth lead, $p \neq j$, has the form $s_{pj}e^{ikx}$. Coefficients s_{pj}

are entries of the scattering matrix. As for the curved edges, the magnetic field leads to appearance of additional phase (see above) for exponential terms. But this phase does not depend on the spectral parameter k. Correspondingly, the behavior of the determinant of the scattering matrix at infinity (which is important for the completeness) does not change essentially, and the proof follow the same way as for the Schrödinger operator without a magnetic field. The linear system for determination of s_{pj} and coefficients of the solutions for edges is given by the Dirichlet condition at boundary vertices, continuity at each non-boundary vertex, the Kirchhoff condition (3.1) at each non-boundary vertex. For each jth incoming wave, one obtains a linear algebraic system for the coefficients, i.e., the number of systems coincides with the number of semi-infinite leads of Γ.

3.2. Graph containing balanced vertices

As has been described, the problem of scattering matrix construction reduces to the inhomogeneous linear system for the coefficients, having units in the right hand side of two equations and zeros at the right hand side of others. It is convenient to reorder the equations in the system by the following way. Let us take an external vertex v coupling m edges and m leads (balanced). Let the first m equations correspond to continuity condition for leads, the next m equations to continuity condition for edges, $(2m+1)$th equation to the Kirchhoff condition for the vertex. As for internal vertices, the order of the corresponding equations can be arbitrary because the scattering matrix includes the first m coefficients only. The term s_{pj} of the scattering matrix is the pth coefficient of the jth system. Kramer's formula gives one the system solution as a ratio of two determinants. The system matrix consists of $0, 1$ and exponentials of type $e^{\pm ikL_s+i\Phi_s}$ where L_s is the length of the sth edge and Φ_s is the additional phase due to the magnetic field. For the chosen external balanced vertex, one has the matrix of the corresponding part of the system in the following block form (due to the chosen ordering of the equations)

$$A = \begin{pmatrix} B & C \\ D & E \end{pmatrix}$$

where B is a $(2m+1)\times(2m+1)$ matrix. The determinant $\det A$ has the form of exponential polynomial

$$\sum_{r=1}^{n} a_r e^{ik\sigma_r} \tag{3.1}$$

where $\sigma_r \in \mathbb{R}$, a_r is a polynomial in k. We denote $\sigma^- = \min\{\sigma_1,\dots,\sigma_n\}$ and $\sigma^+ = \max\{\sigma_1,\dots,\sigma_n\}$. It is these coefficients that predetermine the behavior (exponential in k or power in k) of the determinant for large $|\Im k|$. This, in its turn, allows us to estimate the integral in the completeness criterion.

Let us consider the determinant at the denominator of the Kramer formula. The determinant is the sum of the products of entries of A where every column contributes one entry to each product. In order for the product to be of the type $a^- e^{ik\sigma_-}$, each column corresponding to an "edge" e_s variable must contribute the entry e^{-ikL_s}. We are interested in the term with the maximal exponential growth only. Correspondingly, other terms can be ignored. It will be made if we replace the constant entries of the columns by zeros. This will not affect the value of $a^-(\det A)$ (recall that a^- is the coefficient of the term with the maximal exponential growth). However, the columns of D corresponding to the "leads" variables are all zeros. Hence, we come to the conclusion that

$$a^-(\det A) = a^-(\det A_0), \quad A_0 = \begin{pmatrix} B & C \\ 0 & E \end{pmatrix}.$$

Note that $\det A_0 = \det B \det E$. As for B, one can see that simple row reduction shows that $\det B = 0$ for a balanced vertex. It means that the coefficient $a^-(\det A)$ vanishes.

The determinant in the numerator of the Kramer formula differs from the previous one in one column which is replaced by the column of the right hand side terms of the system. Really, it means that we replace only one entry – unit in the row corresponding to the Kirchhoff condition by zero. In this case, the same row reduction as above shows that $a_-(\det A) \neq 0$. As a result, the determinants ratio contains an exponential factor. It concerns to the block related to vertex v. Other entries of the columns of the scattering matrix related to these input-output leads has the exponential factor too due to the same reasons as above. Hence, the determinant of the scattering matrix has this exponential factor. It is a non-identical singular inner factor for the scattering matrix factorization. Correspondingly, the system of resonance states is not complete if the graph has balanced external vertices in accordance with the completeness criterion (the scattering matrix is not a Blaschke–Potapov product).

Remark 3.2. One can see that there is no need to consider the integral in the completeness criterion in this case although it can be made simply. It is clear for this case, that $\ln s(k)$ has linear growth in the upper half-plane due to the presence of an exponential factor in $s(k)$. Consequently, the corresponding integral does not tend to zero for $\mathsf{R} \to \infty$.

3.3. Graph containing only unbalanced vertices

Consider the case when all external vertices are unbalanced. Let for jth external vertex one have m_j leads and p_j edges ($m_j \neq p_j$ for any j). We can prove the completeness using induction in number of external vertices. The system matrix for the case of j leads has the form

$$A_j = \begin{pmatrix} B_j & C_j \\ D_j & E_j \end{pmatrix}.$$

To organize the induction procedure, we take into account that the matrix A_{j-1} is obtained from corresponding matrix A_j by deleting the columns corresponding to variables of jth lead, and rows corresponding to leads related to jth vertex. Analogously to the previous section, we find that the main term of the corresponding block of the determinant from the denominator of the Kramer formula is as follows:

$$a_j^- = a^-(\det B_j \det E_j)$$

and

$$a_{j-1}^- = a^-(\det B_{j-1} \det E_{j-1}).$$

Reduction of rows shows that

$$\det B_j = (m_j - p_j)e^{-ik(L_1+L_2+\cdots+L_j)}, \quad \det B_{j-1} = -p_(m_j - p_j)e^{-ik(L_1+L_2+\cdots+L_j)}.$$

One can see that if $a_{j-1}^- \neq 0$ then $a_j^- \neq 0$. Thus, by induction, one gets the nonzero main term in the denominator. The determinant in the numerator has the nonzero main term $a_j^- \neq 0$. Hence, the numerator and denominator from the Kramer formula have the same order in the upper half-plane (and in the lower half-plane, too), hence, the determinant of the scattering matrix is of order 1 and has no exponential factor. This means that the scattering matrix is the Blaschke–Potapov product, correspondingly, the system of resonance states is complete in $L_2(\Gamma_0$. The formal proof based on the criterion (2.5) is presented in Appendix.

Remark 3.3. Taking into account Theorem 2.4, one can simply obtain the following Corollary from the main Theorem 2.15: The system of resonance states is complete on $L^2(\Gamma_0)$ if and only if the resonances have the Weyl asymptotics, i.e., Γ is a Weyl graph. It is the same issue as for the Schrödinger operator without a magnetic field. The reasons for the Weyl asymptotics and for the completeness are, in principle, the same: sufficient number of resonance states. The idea that resonances have the Weyl asymptotics if and only if the corresponding resonance states form a complete set in a proper domain seems to be correct for wider class of objects than quantum graphs.

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Appendix

Formal proof of completeness/incompleteness of the resonance states can be obtained by using the criterion (2.5) which reduces the problem to estimation of the following integral

$$\int_0^{2\pi} F(t)dt = \int_0^{2\pi} \frac{\mathsf{R}(r)\ln(s(\mathsf{R}(r)e^{it} + i\mathsf{C}(r)))}{(\mathsf{R}(r)e^{it} + i\mathsf{C}(r) + i)^2} dt.$$

Here C, R are given by (2.6), $s = |\det S|$. For balanced and unbalanced cases one obtains different results. If all external vertices are unbalanced, one has completeness of the resonance states, if there is a balanced vertex (or several balanced vertices), one obtains the incompleteness. As for the last case, it has been considered above.

Let all external vertices be unbalanced. It has been proved in the previous section that $\ln s(k)$ is of order $O(1)$ for $k \to \infty$, $y = \Im k > 0$, $k = x + iy$.

To estimate the integral, we make a partition of the integration curve. The first part is that inside a strip $0 < y < \delta$. Taking into account that at the real axis ($y = 0$) one has $s(k) = 1$, one obtains $|\ln s(\mathsf{R}e^{it} + \mathsf{C}i)| < \delta$. The length of the corresponding part of the circle is of order $\sqrt{2\mathsf{R}\delta}$. As a result, the integral over this part of the curve is $o(1/\sqrt{\mathsf{R}})$ and tends to zero if $\mathsf{R} \to \infty$.

The second part of the integral is related to the singularities of F, i.e., the roots of $s(k)$ (resonances). In our case the determinant has a form of quasi-polynomial (3.1). The distribution of roots of such quasi-polynomials were studied in many works during a long time [34, 35, 36, 37]. The roots are posed along logarithmic curves in the complex plane. We need only a small part of this information. First, that these values are roots of an analytic function. Correspondingly, the number of roots at the integration curve is finite. Moreover, we know [28] that for such quantum graph, one has the Weyl asymptotics of the resonances, but at this step we need not this detailed information. Let t_0 be the value of a parameter corresponding to a resonance. Let us take a vicinity $(t_0 - \delta_1', t_0 + \delta_1)$ such that outside it we have

$$|\ln s(\mathsf{R}e^{it} + \mathsf{C}i)| < c_1. \tag{3.2}$$

Inside the interval, we have

$$|F| \leq c_2 \mathsf{R}^{-1} \ln t.$$

The corresponding integral is estimated as

$$I_2 = \left| \int_{t_0 - \delta_1'}^{t_0 + \delta_1} F(t) dt \right| \leq c_2 \mathsf{R}^{-1} \delta_1 \ln \delta_1.$$

On the remaining part of the integration curve we have $|F| \leq c_1 \mathsf{R}^{-1}$, and the length of the integration interval is not greater than 2π.

Thus, the procedure of estimation is as follows. Choose δ_1', δ_1 to separate the root (or roots) of $s(k)$. If $t_0 - \delta_1 > 0$ then consider $(0, t_0 - \delta_1]$ separately (for the second semi-circle $\pi \leq t < 2\pi$ the consideration is analogous). For this part of the curve with small t (i.e. small y), the estimation of the integral is $O(1/\sqrt{\mathsf{R}})$. For the part of the curve outside these intervals, the estimation of the integral is $O(1/\mathsf{R})$. Consequently, the full integral is estimated as $O(1/\sqrt{\mathsf{R}})$, i.e., the integral tends to zero if $\mathsf{R} \to \infty$. In accordance with the completeness criterion we have the completeness in this case.

Thus, the proof is complete.

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On $\mathbb{Z}_d$-symmetry of spectra of some nuclear operators

Oleg Reinov

This paper is dedicated to the memory of one of the wonderful mathematicians and my best teachers, Prof. Boris Pavlov.

Abstract. It was shown by M.I. Zelikin (2007) that the spectrum of a nuclear operator in a Hilbert space is central-symmetric iff the traces of all odd powers of the operator equal zero. B. Mityagin (2016) generalized Zelikin's criterium to the case of compact operators (in Banach spaces) some of which powers are nuclear, considering even a notion of so-called $\mathbb{Z}_d$-symmetry of spectra introduced by him. We study α-nuclear operators generated by the tensor elements of so-called α-projective tensor products of Banach spaces, introduced in the paper (α is a quasi-norm). We give exact generalizations of Zelikin's theorem to the cases of $\mathbb{Z}_d$-symmetry of spectra of α-nuclear operators (in particular, for s-nuclear and for (r,p)-nuclear operators). We show that the results are optimal.

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1. Introduction

It is well known that every nuclear (= trace class) operator on a Hilbert space has the absolutely summable sequence of eigenvalues [21]. Moreover, the famous Lidskiĭ theorem [11] says that for such an operator its trace is equal to the sum of all its eigenvalues (written in according to their algebraic multiplicities).

It is clear that if the spectrum of such an operator is central-symmetric, then its trace equals zero. Moreover, since every power of a nuclear operator T is nuclear too and has a central-symmetric spectrum if T has, we see that, for such T, trace $T^k = 0$ for every odd natural number k.

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M.I. Zelikin has noticed that for an finite dimensional spaces the converse is also true (see [23, Theorem 1]), and then he proved the corresponding theorem for any nuclear operator in a separable Hilbert space ([23, Theorem 2]). At the same time, his proof was rather complicated. We are going to present, in particular, a more simple proof below.

Recall that the spectrum of a compact operator is central-symmetric, if together with any eigenvalue $\lambda \neq 0$ it has the eigenvalue $-\lambda$ of the same multiplicity. Thus, M.I. Zelikin has proved that the spectrum of a nuclear operator A acting on a separable Hilbert space is central-symmetric iff trace $A^{2n-1} = 0, \forall n \in \mathbf{N}$.

Let us mention that this theorem cannot be extended to the case of general Banach spaces: it follows from Grothendieck–Enflo–Davie results [7, 4, 3] that there exists a nuclear operator T in the space l_1 of absolutely summable sequences such that $T^2 = 0$ but trace $T = 1$ (the operator can be chosen even in such a way that it is s-nuclear for every $s \in (2/3, 1]$; see Definition 1 below and [13, 10.4.5]).

A right generalization of Zelikin's theorem was found by B. Mityagin [12]. He introduced a notion of so-called Z_d-symmetry of the spectra of compact operators in Banach spaces and gave a criterium for the spectra of an operator (some of which power is nuclear) to be Z_d-symmetric. For $d = 2$, this gives a generalization of the criterium of M.I. Zelikin. We will use this notion of the Z_d-symmetry to formulate and to prove an *exact* generalization of Zelikin's theorem for the case of subspaces of quotients of L_p-spaces (thus getting, in a simpler way, Zelikin's result putting $p = 2$ and $d = 2$). However, we will have to consider so-called s-nuclear operators instead of nuclear ones in Zelikin's theorem. To formulate our main result, let us recall the definitions of s-nuclearity of operators and of Z_d-symmetry of spectra.

Definition 1.1 (A. Grothendieck). *An operator $T : X \to Y$ is s-nuclear $(0 < s \leq 1)$ if*

$$\exists\ (x'_k) \subset X^*, (y_k) \subset Y : \sum_{k=1}^{\infty} ||x'_k||^s \, ||y_k||^s < \infty, \quad T(x) = \sum_{k=1}^{\infty} x'_k(x) y_k, \quad \forall\ x \in X.$$

For $s = 1$, we say that T is nuclear.

Let us note that A. Grothendieck in [7] called such operators "applications de puissance p.éme sommable".

Definition 1.2 (B. Mityagin). *Let T be an operator in X, all non-zero spectral values of which are eigenvalues of finite multiplicity and have no limit point except possibly zero. For a fixed $d = 2, 3, \ldots$ and for the operator T, the spectrum of T is called $\mathbb{Z}_d$-symmetric, if $0 \neq \lambda \in \mathrm{sp}\,(T)$ implies $t\lambda \in \mathrm{sp}\,(T)$ for every $t \in \sqrt[d]{1}$ and of the same multiplicity.*

Our generalization of the Zelikin's theorem is:

Theorem 1.1. *Let Y be a subspace of a quotient (or a quotient of a subspace) of some $L_p(\mu)$-space, $1 \leq p \leq \infty$ and $1/r = 1 + |1/2 - 1/p|$. If $T : Y \to Y$ is r-nuclear, then* trace T *is well-defined. For a fixed $d = 2, 3, \ldots$, the spectrum of T*

is $\mathbb{Z}_d$*-symmetric iff* trace $T^{kd+j} = 0$ *for all* $k = 0, 1, 2, \dots$ *and* $j = 1, 2, \dots, d-1$. *In particular, if* trace $T \neq 0$, *then* $T^2 \neq 0$.

Note that if $d = 2$, we obtain an exact generalization of Zelikin's theorem on the central symmetry.

Also, we present some sharp (optimal in r, p) generalizations of Zelikin's theorem to the case of so-called (r, p)-nuclear and dually (r, p)-nuclear operators (see Theorem 4.2).

Theorems 1.1 and 4.2 are optimal with respect to p and r :

Theorem 1.2. *Let* $p \in [1, \infty], p \neq 2$, $1/r = 1 + |1/2 - 1/p|$. *There exists a nuclear operator* V *in* l_p (*in* c_0 *for* $p = \infty$) *such that*

(1) V *is* s*-nuclear for each* $s \in (r, 1]$;
(2) V *is not* r*-nuclear;*
(3) trace $V = 1$ *and* $V^2 = 0$.

Note that for $p = \infty$ or $p = 1$ we have $r = 2/3$ and for $p = 2$ we have $r = 1$. The proofs will be given in Sects. 4.5 and 4.6

Let us note that some of the implications of our results on $\mathbb{Z}$-symmetry of spectra are the consequences of Mityagin's theorem. But it seems that our proofs are shorter. Besides, our aim was to obtain the *exact* generalizations of Zelikin's theorem in an independent way.

2. Content

In Sect. 3, we present the general notations concerning Banach spaces, spaces of operators, tensor products, vector-valued sequence spaces.

In Sect 4.1, we give a definition of projective tensor quasi-norms α and introduce the α-projective tensor products of Banach spaces. We show that these tensor products are continuously imbedded in the projective products of A. Grothendieck. For complete α-projective tensor products, we define α-nuclear operators in a natural way (as elements of corresponding factor spaces). Also in a natural way, we define a notion of the approximation property AP_α, give a simple characterization of Banach spaces with this property and present some main examples.

In Sect. 4.2, we consider some properties of the α-projective tensor products of spectral type l_1 (so that all α-nuclear operators have absolutely summable sequences of their eigenvalues). In particular, we are interested in the question of when the trace formulas are true. In the end, examples are given.

In Sect. 4.3, we introduce so-called α-extension and α-lifting properties for a projective tensor quasi-norms α. We are interested here in connection between the AP_α, trace formulas and the statements of type "trace $T = 1 \implies T^2 \neq 0$".

In Sect. 4.4, we prove one of the main theorems on $\mathbb{Z}_d$-symmetry of spectra of α-nuclear operators. We apply the results to some concrete quasi-normed tensor products, getting a generalization of Zelikin's theorem to the case of (r, p, q)-nuclear operators in general Banach spaces.

In Sect. 4.5, a proof of Theorem 1.1 is given.

Finally, in Sect. 4.6, we show that the main results of the previous subsections are sharp. Maybe, it worthwhile to mention a new result on the asymptotically Hilbertian spaces (the last theorem in the paper).

3. Notation and preliminaries

Throughout, we denote by $X, Y, E, F, W \dots$ Banach spaces over a field $\mathbb{K}$ (which is either $\mathbb{R}$ or $\mathbb{C}$); $X^*, Y^*, \dots$ are Banach dual to $X, Y, \dots$. By $x, y, x', \dots$ (maybe with indices) we denote elements of $X, Y, X^* \dots$, respectively; $\pi_Y : Y \to Y^{**}$ is a natural isometric imbedding. By a subspace of a Banach space we mean a closed linear subspace.

Notations $l_p, (0 < p \leq \infty, n = 1, 2, \dots)$, c_0 are standard; e_k $(k = 1, 2, \dots)$ is the kth unit vector in l_p or c_0 (when we consider the unit vectors as the linear functionals, we use notation e_k'). We use id_X for the identity map in X.

It is denoted by $F(X, Y)$ a vector space of all linear continuous finite rank mappings from X to Y. By $X \otimes Y$ we denote the algebraic tensor product of the spaces X and Y; $X \otimes Y$ can be considered as a subspace of the vector space $F(X^*, Y)$ (namely, as a vector space of all linear weak*-to-weak continuous finite rank operators). We can identify also the tensor product (in a natural way) with a corresponding subspace of $F(Y^*, X)$. If $X = W^*$, then $W^* \otimes Y$ is identified with $F(W, Y)$. If $z \in X \otimes Y$, then $\widetilde{z}$ is the corresponding finite rank operator. If $z \in X^* \otimes X$ and, e.g., $z = \sum_{k=1}^n x_k' \otimes x_k$, then trace $z := \sum_{k=1}^n \langle x_k', x_k \rangle$ does not depend on representation of z in $X^* \otimes X$; $L(X, Y)$ is a Banach space of all linear continuous mappings ("operators") from X to Y equipped with the usual operator norm.

If $A \in L(X, W)$ and $B \in L(Y, G)$, then a linear map $A \otimes B : X \otimes Y \to W \otimes G$ is defined by $A \otimes B(x \otimes y) := Ax \otimes By$ (and then extended by linearity). Since $\widetilde{A \otimes B(z)} = B \widetilde{z} A^*$ for $z \in X \otimes Y$, we will use notation $B \circ z \circ A^* \in W \otimes G$ for $A \otimes B(z)$. In the case where X is a dual space, say F^*, and $T \in L(W, F)$ (so, $A = T^* : F^* \to W^*$), one considers a composition $B \widetilde{z} T$; in this case $T^* \otimes B$ maps $F^* \otimes Y$ into $W^* \otimes Y$ and we use notation $B \circ z \circ T$ for $T^* \otimes B(z)$.

A projective tensor product $X \widehat{\otimes} Y$ of Banach spaces X and Y is defined as a completion of $X \otimes Y$ with respect to the norm $||\cdot||_\wedge$: if $z \in X \otimes Y$, then $||z||_\wedge := \inf \sum_{k=1}^n ||x_k||\, ||y_k||$, where infimum is taken over all representation of z as $\sum_{k=1}^n x_k \otimes y_k$. We can try to consider $X \widehat{\otimes} Y$ also as operators $X^* \to Y$ or $Y^* \to X$, but this correspondence is, in general, not one-to-one. However, the natural map $(X \otimes Y, ||\cdot||_\wedge) \to L(X^*, Y)$ is continuous and can be extended to the completion $X \widehat{\otimes} Y$; for a tensor element $z \in X \widehat{\otimes} Y$, we still denote by $\widetilde{z}$ the corresponding operator. Note that $X \widehat{\otimes} Y = Y \widehat{\otimes} X$ in a sense. If $z \in X \widehat{\otimes} Y, \varepsilon > 0$, then one can represent z as $z = \sum_{k=1}^\infty x_k \otimes y_k$ with $\sum_{k=1}^\infty ||x_k||\, ||y_k|| < ||z||_\wedge + \varepsilon$. For $z \in X^* \widehat{\otimes} X$ with a "projective representation" $z = \sum_{k=1}^\infty x_k' \otimes x_k$, trace $z := \sum_{k=1}^\infty \langle x_k, y_k \rangle$ does not depend of representation of z. The Banach dual $(X\widehat{\otimes} Y)^*$ equals $L(Y, X^*)$ (with duality $\langle T, z\rangle = \text{trace}\, T\circ z$.)

One more notation: If $\mathfrak{A}$ is an operator ideal [13] then we often use the notation $\mathfrak{A}(X)$ for the space $\mathfrak{A}(X, X)$.

Finally,

$$l_p(X) := \left\{(x_i)\subset X:\ ||(x_i)||_p := \left(\sum ||x_i||^p\right)^{1/p} < \infty\right\},$$

$$l_\infty(X) := \left\{(x_i)\subset X:\ ||(x_i)||_\infty := \sup_i ||x_i|| < \infty\right\},$$

$$l_p^w(X) := \left\{(x_i)\subset X:\ ||(x_i)||_{w,p} := \sup_{||x'||\le 1}\left(\sum |\langle x', x_i\rangle|^p\right)^{1/p} < \infty\right\},$$

$$l_\infty^w(X) := \left\{(x_i)\subset X:\ ||(x_i)||_{w,\infty} := \sup_i ||x_i|| < \infty\right\}.$$

Note that if $p\le q$, then $||\cdot||_q \le ||\cdot||_p$ and $||\cdot||_{w,q}\le ||\cdot||_{w,p}$. If $0<p\le\infty$, then p' is a conjugate exponent: $1/p + 1/p' = 1$ if $p\ge 1$ and $p'=\infty$ if $p\in(0,1]$.

4. Quasi-normed tensor products and approximation properties

4.1. Projective quasi-norms and approximation properties

Let α be a function on a vector space E, $\alpha: E\to\widehat{\mathbb{R}}$. We say that α is a *quasi-norm* on E if (1) $\alpha(E)\subset[0,+\infty]$ and $\alpha(x)=0$ implies $x=0$; (2) there exists a constant $C>0$ such that $\alpha(x+y)\le C\,[\alpha(x)+\alpha(y)]$ for $x,y\in E$; (3) $\alpha(ax) = |a|\,\alpha(x)$ for $a\in\mathbb{K}, x\in E$.

Definition 4.1. (i) *Given a pair (E,α), where α is a quasi-norm on a vector space E, a quasi-normed space associated with the pair (E,α) is the quasi-normed vector space*

$$E_\alpha := \{x\in E:\ \alpha(x)<\infty\}.$$

(ii) *The quasi-normed space E_α is complete (= a quasi-Banach space), if every Cauchy sequence in E_α α-converges to an element of E_α.*

Note that E_α is a quasi-normed vector space in the sense of [9, p. 159] and we may generate the corresponding topology (see [9, p. 159–160], [1, p. 445]).

Remark 4.1. (1) It may be that $E_\alpha = E$.

(2) It is well known [1, p. 445] that if E_α is a quasi-normed space, then there are a number $\beta\in(0,1]$ and a β-norm $||\cdot||$ on E_α which is equivalent to the quasi-norm α. Recall that a β-norm on a vector space F is a quasi-norm $||\cdot||: F\to\mathbb{R}$ such that for all $x,y\in F$ one has the following β-triangle inequality: $||x+y||^\beta \le ||x||^\beta + ||y||^\beta$.

Now, let α be a quasi-norm on a projective tensor product $X\widehat{\otimes}Y$ such that $\alpha(x\otimes y)=||x||\,||y||$ for $x\in X, y\in Y$. The associated quasi-normed tensor product (which will be denoted by $X\widehat{\otimes}_\alpha Y$ and called "α-projective tensor product") is the α-closure of $X\otimes Y$ in $(X\widehat{\otimes}Y)_\alpha$ (in the concrete cases we will use some specific notations). Thus,

$$X\widehat{\otimes}_\alpha Y := \Big\{u\in X\widehat{\otimes}Y:\ \alpha(u)<\infty \ \text{ and } \ \exists\,(u_n)\subset X\otimes Y:\ \alpha(u-u_n)\underset{n\to\infty}{\to} 0\Big\}.$$

More generally:

Definition 4.2. (i) *Let $\widehat{\otimes}$ denotes the class of all tensor elements of the projective tensor products of arbitrary Banach spaces. A projective tensor quasi-norm α is a map from $\widehat{\otimes}$ to $\widehat{\mathbb{R}}$ such that α is a quasi-norm on each component $X\widehat{\otimes}Y$ with the properties:*

(Q_1) $\alpha(x\otimes y)=||x||\,||y||$ *for $x\in X, y\in Y$.*

(Q_2) *There exists a constant $C>0$ such that $\alpha(u_1+u_2)\le C\,[\alpha(u_1)+\alpha(u_2)]$ for all X,Y and $u_1,u_2\in X\widehat{\otimes}Y$.*

(Q_3) *If $u\in X\widehat{\otimes}Y$, $A\in L(X,E)$ and $B\in L(Y,F)$, then $\alpha(A\otimes B(u))\le ||A||\,\alpha(u)\,||B||$.*

(ii) *A projective tensor quasi-norm α is said to be complete, if every α-projective tensor product $X\widehat{\otimes}_\alpha Y$ is complete, that is quasi-Banach.*

For every projective tensor quasi-norm α there exist $\beta\in(0,1]$ and an equivalent β-norm $||\cdot||_\beta$ on $\widehat{\otimes}$ so that $X\widehat{\otimes}_\alpha Y = X\widehat{\otimes}_{||\cdot||_\beta}Y$ (i.e., there exists a quasi-norm $||\cdot||_\beta$ with β-triangle inequality such that for some positive constants C_1,C_2 and for all projective tensor elements u the inequalities $C_1\alpha(u)\le ||u||_\beta\le C_2\alpha(u)$ hold). Thus, we may assume, if needed, that a priori α is a β-norm.

We are not going to consider here in detail the properties of just introduced objects. But we need below the fact that the inclusions $X\widehat{\otimes}_\alpha Y\hookrightarrow X\widehat{\otimes}Y$ are continuous for all Banach spaces X,Y (in the main Example 4.1 below this will be automatically fulfilled).

Proposition 4.1. *Let α be a complete projective tensor norm. The natural injections $X\widehat{\otimes}_\alpha Y\to X\widehat{\otimes}Y$ are continuous for all Banach spaces X and Y. Moreover, there is a constant $d=d(\alpha)$ such that for all X, Y and $u\in X\widehat{\otimes}_\alpha Y$ we have: $||u||_\wedge\le d\,\alpha(u)$.*

Proof. Suppose the last assertion is not true and there exist sequences $(X_n),(Y_n)$ and (u_n) with $u_n\in X_n\widehat{\otimes}_\alpha Y_n$ so that $\alpha(u_n)\le 1/(2C)^n$ and $||u_n||_\wedge\ge n$. Put $X:=\big(\sum X_n\big)_{l_2}$ and $Y:=\big(\sum Y_n\big)_{l_2}$. Let $i_n: X_n\to X$ and $j_n: Y_n\to Y$ be the natural injections. Consider the sequence $(z_N):=\big(\sum_{k=1}^N(i_k\otimes j_k)(u_k)\big)$. For any natural numbers K and m, we have:

$$\alpha\Big(\sum_{k=K+1}^{K+m}(i_k\otimes j_k)(u_k)\Big)\le\sum_{k=1}^{m}C^k\,\alpha\big((i_{K+k}\otimes j_{K+k})(u_{K+k})\big)$$
$$\le\sum_{k=1}^{\infty}\frac{C^k}{(2C)^{K+k}}\le\frac{1}{(2C)^K}.$$

Hence, (z_N) is a Cauchy sequence in $X\widehat{\otimes}_\alpha Y$ and, by the completeness of α, converges to an element $u:=\sum_{k=1}^{\infty}(i_k\otimes j_k)(u_k)\in X\widehat{\otimes}_\alpha Y$. On the other hand, if $P_n: X\to X_n$ and $Q_n: Y\to Y_n$ are the natural "projections", then $||u||_\wedge\ge ||(P_n\otimes Q_n)(u)||_\wedge=||u_n||_\wedge\ge n$. □

Since $X\widehat{\otimes}_\alpha Y$ ia a linear subspace of $X\widehat{\otimes}Y$, the space $L(Y,X^*)$ separates points of $X\widehat{\otimes}_\alpha Y$. If $u\in X\widehat{\otimes}_\alpha Y$, then $u=0$ iff trace $U\circ u=0$ for every $U\in L(Y,X^*)$. In particular, the dual space $(X\widehat{\otimes}_\alpha Y)^*$ separates points of $X\widehat{\otimes}_\alpha Y$.

It is clear that every tensor element $u\in X\widehat{\otimes}_\alpha Y$ generates a nuclear operator $\widetilde{u}: X^*\to Y$. If X is a dual space, say E^*, then we get a canonical mapping $j_\alpha: E^*\widehat{\otimes}_\alpha Y\to L(E,Y)$. The image of j_α is denoted here by $N_\alpha(E,Y)$, and we equip it with an "α-nuclear" quasi-norm ν_α : This is a quasi-norm induced from $E^*\widehat{\otimes}_\alpha Y$ via the quotient map $E^*\widehat{\otimes}_\alpha Y\to N_\alpha(E,Y)$. If the projective tensor quasi-norm α is complete, then $N_\alpha(E,Y)$ is a quasi-Banach space.

Definition 4.3. *Let α be a complete projective tensor quasi-norm. We say that a Banach space X has the approximation property AP_α, if for every Banach space E the canonical map $E^*\widehat{\otimes}_\alpha X\to N_\alpha(E,X)$ is one-to-one (in other words, if $E^*\widehat{\otimes}_\alpha X=N_\alpha(E,X)$).*

Note that if $\alpha=||\cdot||_\wedge$, then we get the classical approximation property AP of A. Grothendieck [7]. It must be clear that the AP implies the AP_α, for any projective tensor quasi-norm.

We will need below the following

Lemma 4.1. *A Banach space X has the AP_α iff the canonical map $X^*\widehat{\otimes}_\alpha X\to L(X)$ is one-to-one.*

Proof. It is enough to repeat (word for word with same notations) the proof of [20, Proposition 6.1]. □

Example 4.1. Let $0<r,s\le 1$, $0<p,q\le\infty$ and $1/r+1/p+1/q=1/\beta\ge 1$. We define a tensor product $X\widehat{\otimes}_{r,p,q}Y$ as a linear subspace of the projective tensor product $X\widehat{\otimes}Y$, consisting of all tensor elements z which admit representations of type

$$z=\sum_{k=1}^{\infty}\alpha_k x_k\otimes y_k,\quad (\alpha_k)\in l_r,\ (x_k)\in l_{w,p}(X),\ (y_k)\in l_{w,q}(Y); \tag{1}$$

we equip it with the quasi-norm $||z||_{r,p,q}:=\inf||(\alpha_k)||_r\,||(x_k)||_{w,p}\,||(y_k)||_{w,q}$, where the infimum is taken over all representations of z in the above form (1). Note that this tensor product is β-normed (cf. [10], where it is considered a "finite-sums-representation" version of the above tensor product). It is quasi-Banach (for the completeness, see the author's preprint "Approximation properties associated with quasi-normed operator ideals of (r,p,q)-nuclear operators"[1]). The corresponding quasi-normed operator ideal $N_{r,p,q}$ is the quasi-Banach ideal of (r,p,q)-nuclear operators (cf. [13, 10]). In particular cases where one or two of the exponents p,q are ∞, we will use the notations close to those from [18, 20] (here we change p',q' to p,q) : We denote $N_{r,\infty,\infty}$ by N_r, $N_{r,\infty,q}$ by $N_{[r,q]}$, $N_{r,p,\infty}$ by $N^{[r,p]}$, $\widehat{\otimes}_{r,\infty,\infty}$ by $\widehat{\otimes}_r$, $\widehat{\otimes}_{r,\infty,q}$ by $\widehat{\otimes}_{[r,q]}$, $\widehat{\otimes}_{r,p,\infty,}$ by $\widehat{\otimes}^{[r,p]}$.

The corresponding notations are used also for the $AP_{r,p,q}$:

(i) For $p=q=\infty$, we get the AP_r from [20].
(ii) For $p=\infty$, we get the $AP_{[r,q]}$ from [18, 20].
(iii) For $q=\infty$, we get the $AP^{[r,p]}$ from [18, 20].

We will need some known facts concerning the approximation properties from Example 4.1. Let us collect them in

Lemma 4.2. (1) [16, Corollary 10] *Let $s\in(0,1]$, $p\in[1,\infty]$ and $1/s=1+|1/p-1/2|$. If a Banach space Y is isomorphic to a subspace of a quotient (or to a quotient of a subspace) of an L_p-space then it has the property AP_s.*
(2) [18, Corollary 4.1], [20, Theorem 7.1] *Let $1/r-1/p=1/2$. Every Banach space has the properties $AP_{[r,p']}$ and $AP^{[r,p']}$.*

A proof of the assertion (2) can be found below (see Example 4.3). See also [20] for some other results in this direction.

Remark 4.2. *As a matter of fact, a proof of the assertion that every Banach space has the $AP^{[1,2]}$ is contained implicitly in* [13]*. It was obtained also there that this assertion (after applying some results of Complex Analysis) implies the Grothendieck–Lidskiĭ type trace formulas for operators from $N^{[1,2]}$* [13, 27.4.11] *(and this implies the Lidskiĭ trace formula for trace-class operators in Hilbert spaces and the Grothendieck trace formula for $N_{2/3}$ as well). On the other hand, there is a very simple way to get these results on $AP^{[1,2]}$ and $N^{[1,2]}$ from the Lidskiĭ theorem (see the proofs of* [20, Theorems 7.1–7.3] *for $p=2$).*

4.2. Spectral type l_1

Let T be an operator in X, all non-zero spectral values of which are eigenvalues of finite multiplicity and have no limit point except possibly zero. Put $\lambda(T)=\{\lambda\in \text{eigenvalues}\,(T)\setminus\{0\}\}$ (the eigenvalues of T are taken in according to their multiplicities). We say that an operator $T\in L(X,X)$ is *of spectral type* l_1, if the sequence of all eigenvalues $\lambda(T):=(\lambda_k(T))$ is absolutely summable. In this case, we can define the *spectral trace of* T : $\operatorname{sp\,tr}(T):=\sum\lambda_k(T)$. We say that a subspace $L_1(X,X)\subset L(X,X)$ is *of spectral type* l_1, if every operator $T\in L_1(X,X)$ is of spectral type l_1. Recall that an operator ideal $\mathfrak{A}$ is of spectral type l_1, if every its component $\mathfrak{A}(X,X)$ is of spectral type l_1.

[1] http://www.mathsoc.spb.ru/preprint/2017/index.html#08

Definition 4.4. *Let α be a projective tensor quasi-norm. The tensor product $X\widehat{\otimes}_\alpha X$ is of spectral type l_1, if the space $N_\alpha(X,Y)$ is of spectral type l_1. The projective tensor quasi-norm α (or the tensor product $\widehat{\otimes}_\alpha$) is of spectral type l_1, if the corresponding operator ideal N_α is of spectral type l_1.*

Example 4.2. $N_1(H)$ $(= N_{[1,2]}(H) = N^{[1,2]}(H) = S_1(H)$, trace class operators in a Hilbert space) is of spectral type l_1 [21]. $\widehat{\otimes}_{2/3}$ and $N_1 \circ N_1$ are of spectral type l_1 [7]. $N^{[1,2]}$ is of spectral type l_1 (see [13, see 27.4.9, end of the proof]). $N_{[1,2]}$ is of spectral type l_1 (see [20, Theorem 7.2 for $p = 2$]; it follows also from the previous assertion). More general, if $1/r - 1/p = 1/2$, then $\widehat{\otimes}_{[r,p]} = N_{[r,p]}$, $\widehat{\otimes}^{[r,p]} = N^{[r,p]}$ and they are of spectral type l_1 (see [20, Theorems 7.1–7.3]; a simple proof will be given below in Example 4.3).

Let us note that in all cases in Example 4.2 the trace formula for corresponding operators (say, T) is valid: trace $T = \operatorname{sp\,tr} T$. A general result in this direction is

Proposition 4.2. *Let α be a complete projective tensor quasi-norm of spectral type l_1. For every Banach space X with the AP_α and every $T \in N_\alpha(X)$, one has:* trace $T = \operatorname{sp\,tr} T$. *Conversely, if for a Banach space X and for every $z \in X^*\widehat{\otimes}_\alpha X$ the equality* trace $z = \operatorname{sp\,tr} \widetilde{z}$ *holds, then X possesses the AP_α.*

Proof. Let X has the AP_α. Since the ideal N_α is quasi-Banach and of spectral type l_1, by White's theorem [22, Theorem 2.2] the spectral trace is linear and continuous on N_α. On the other hand, by Proposition 4.1 the usual (nuclear) trace is continuous on $X^*\widehat{\otimes}_\alpha X$, which can be identified with $N_\alpha(X)$ by assumption about X. Since the tensor product $X^* \otimes X$ is dense in $X^*\widehat{\otimes}_\alpha X$, we obtain that trace $T = \operatorname{sp\,tr} T$.

Now, suppose that X does not have the AP_α. By Lemma 4.1, there exists an element $z \in X^*\widehat{\otimes}_\alpha X$ such that trace $z = 1$ and $\widetilde{z} = 0$. By assumptions, $\operatorname{sp\,tr} \widetilde{z} =$ trace $z = 1$. Contradiction. □

Example 4.3. *Let* $0 < r \leq 1$, $1 \leq p \leq 2$, $1/r = 1/2 + 1/p$.

(1) *If $T \in N_{[r,p']}(X)$ (see Example 4.1), then T admits a factorization*

$$T = BA : X \xrightarrow{A} l_p \xrightarrow{B} X, \quad A \in N_r(X, l_p),\ B \in L(l_p, X).$$

The complete systems of eigenvalues of $T = BA$ and AB are the same. But $AB \in N_r(l_p, l_p)$. Therefore, AB is of spectral type l_1, as any r-nuclear operator in l_p [8, Theorem 7]*. It follows from this that $N_{[r,p']}$ is of spectral type l_1. It is easy to see that if $z \in X^*\widehat{\otimes}_{[r,p']}X$ such that $\widetilde{z} = T$, then* trace $z =$ trace AB *(recall that l_p has the AP). But* trace $AB = \operatorname{sp\,tr} AB$ *(it was shown, e.g., in* [19, 20] *and follows also from Proposition 4.2). Hence, for each $z \in X^*\widehat{\otimes}_{[r,p']}X$ we have:* trace $z = \operatorname{sp\,tr} \widetilde{z}$. *By the second part of Proposition 4.2, every Banach space has the property $AP_{[r,p']}$ $(= AP_{r,\infty,p'}$, see Example 4.1; thus, we gave a proof of Lemma 4.2(2) for the case of $AP_{[r,p']}$).*

(2) *If* $T \in N^{[r,p']}(X)$ *(see Example* 4.1*), then* T *admits a factorization*

$$T = BA : X \xrightarrow{A} l_p \xrightarrow{B} X, \quad A \in L(X, l_p),\ B \in N_r(l_p, X).$$

As in (1), we see that for each $z \in X^* \widehat{\otimes}^{[r,p']} X$ *we have:* $\operatorname{trace} z = \operatorname{sp\,tr} \widetilde{z}$. *Furthermore, by the second part of Proposition* 4.2*, every Banach space has the property* $AP^{[r,p]}$ $(= AP^{r,\infty,p'}$, *see Example* 4.1*; thus, we have a proof of Lemma* 4.2(2) *for the case of* $AP^{[r,p']}$).

4.3. α-extension property and α-lifting property

We give now two definitions, which will be of use below. Let us note that these definitions can be generalized in many different ways.

Definition 4.5. *Let* α *be a complete projective tensor quasi-norm. A Banach space* X *has the* α*-extension property, if for any subspace* $X_0 \subset X$ *and every tensor element* $z_0 \in X_0^* \widehat{\otimes}_\alpha X_0$ *there exists an extension* $z \in X^* \widehat{\otimes}_\alpha X_0$ *(so that* $z \circ i = z_0$ *and* $\operatorname{trace} i \circ z = \operatorname{trace} z_0$, *where* $i : X_0 \to X$ *is the natural injection). A Banach space* X *has the* α*-lifting property, if for every subspace* X_0 *and every tensor element* $z_0 \in (X/X_0)^* \widehat{\otimes}_\alpha X/X_0$ *there exists a lifting* $z \in (X/X_0)^* \widehat{\otimes}_\alpha X$ *(so that* $Q \circ z = z_0$, *where* Q *is a quotient map from* X *onto* X/X_0, *and* $\operatorname{trace} z \circ Q = \operatorname{trace} z_0$).

Example 4.4. *For instance, every Banach space has the* $||\cdot||_{r,\infty,q}$*-extension property and* $||\cdot||_{r,p,\infty}$*-lifting property (see Example* 4.1*). For the tensor products* $(\widehat{\otimes}_s, ||\cdot||_{s,\infty,\infty})$, $s \in (0,1]$, *all Banach spaces have both the* $||\cdot||_{s,\infty,\infty}$*-extension and* $||\cdot||_{s,\infty,\infty}$*-lifting properties. This follows from Hahn–Banach theorem and from definition of Banach quotients.*

Proposition 4.3. *Let* α *be a complete projective tensor quasi-norm and* X *have the* α*-extension property. Suppose that* X *possesses the* AP_α*, but there exists a subspace* $X_0 \subset X$ *without the* AP_α*. There exists an operator* $S \in N_\alpha(X)$ *such that* $\operatorname{trace} S = 1$ *and* $S^2 = 0$.

Proof. Take $z_0 \in X_0 \widehat{\otimes}_\alpha X_0$ with $\operatorname{trace} z_0 = 1$ and $\widetilde{z}_0 = 0$ (we use Lemma 4.1). By assumption, there exists $z \in X^* \widehat{\otimes}_\alpha X_0$ such that $z_0 = z \circ i$ and $\operatorname{trace} i \circ z = 1$, where $i : X_0 \to X$ is an inclusion. Here is a diagram for the operators:

$$X_0 \xrightarrow{i} X \xrightarrow{\widetilde{z}} X_0 \xrightarrow{i} X. \tag{2}$$

Now, X has the AP_α. Therefore, we can identify the operator $S := \widetilde{i \circ z}$ with the tensor element $i \circ z$. It is clear that $\operatorname{trace} S = 1$ and $S^2 = 0$. □

The following proposition is a strengthening of Proposition 4.2 in an important case.

Proposition 4.4. *Let* α *be a complete projective tensor quasi-norm of spectral type* l_1 *and* X *have the* α*-extension property. If for every* $z \in X^* \widehat{\otimes}_\alpha X$ *the equality* $\operatorname{trace} z = \operatorname{sp\,tr} \widetilde{z}$ *holds, then every subspace* X_0 *of* X *possesses the* AP_α*. Consequently, for every* $T \in N_\alpha(X_0)$*, one has:* $\operatorname{trace} T = \operatorname{sp\,tr} T$.

Proof. Firstly, note that by Proposition 4.2 X has the AP_α. Let X_0 be a subspace of X, $i : X_0 \to X$ be an inclusion map and $z_0 \in X_0^* \widehat{\otimes}_\alpha X_0$ with trace $z_0 = 1$. Take an extension $z \in X^* \widehat{\otimes}_\alpha X_0$ (as in Definition 4.5; hence, $\widetilde{z}\big|_{X_0} = \widetilde{z}_0$ and trace $i \circ z =$ trace z_0) and consider the operators $\widetilde{i \circ z} : X \to X$ and $\widetilde{z \circ i} : X_0 \to X_0$ (see the diagram (2)). By the principle of related operators [13, 27.3.3], $\operatorname{sp\,tr} \widetilde{i \circ z} = \operatorname{sp\,tr} \widetilde{z \circ i}$. By assumption, $\operatorname{sp\,tr} \widetilde{i \circ z} = \operatorname{trace} i \circ z$ Now, since X has the AP_α, it follows from the equality trace $i \circ z =$ trace z_0 that

$$1 = \operatorname{trace} z_0 = \operatorname{sp\,tr} \widetilde{i \circ z} = \operatorname{sp\,tr} \widetilde{z \circ i} = \operatorname{sp\,tr} \widetilde{z}_0.$$

Therefore, $\widetilde{z}_0 \neq 0$. By Lemma 4.1, X_0 has the AP_α. The last statement follows from the first part of Proposition 4.2. □

The following propositions are in a sense dual the previous ones.

Proposition 4.5. *Let α be a complete projective tensor quasi-norm and X have the α-lifting property. Suppose that X possesses the AP_α, but there exists a factor space X/X_0 ($X_0 \subset X$) without the AP_α. There exists an operator $S \in N_\alpha(X)$ such that* trace $S = 1$ *and* $S^2 = 0$.

Proof. Take $z_0 \in X/X_0 \widehat{\otimes}_\alpha X/X_0$ with trace $z_0 = 1$ and $\widetilde{z}_0 = 0$ By assumption, there exists $z \in (X/X_0)^* \widehat{\otimes}_\alpha X$ such that $Q \circ z = z_0$, where Q is a factor map from X onto X/X_0, and trace $z \circ Q =$ trace $z_0 = 1$. Here is a diagram for the operators:

$$X \xrightarrow{Q} X/X_0 \xrightarrow{\widetilde{z}} X \xrightarrow{Q} X/X_0 \xrightarrow{\widetilde{z}} X. \tag{3}$$

Now, X has the AP_α. Therefore, we can identify the operator $S := \widetilde{z \circ Q}$ with the tensor element $z \circ Q$. It is clear that trace $S = 1$ and $S^2 = 0$. □

Proposition 4.6. *Let α be a complete projective tensor quasi-norm of spectral type l_1 and X have the α-lifting property. If for every $z \in X^* \widehat{\otimes}_\alpha X$ the equality* trace $z =$ sp tr $\widetilde{z}$ *holds, then every quotient X/X_0 of X possesses the AP_α. Consequently, for every $T \in N_\alpha(X/X_0)$, one has:* trace $T =$ sp tr T.

Proof. By Proposition 4.2, X has the AP_α. Let X_0 be a subspace of X, $Q : X \to X/X_0$ be a factor map and $z_0 \in (X/X_0)^* \widehat{\otimes}_\alpha X/X_0$ with trace $z_0 = 1$. Take a lifting $z \in (X/X_0)^* \widehat{\otimes}_\alpha X$ (as in Definition 4.5; hence, $Q \circ z = z_0$, and trace $z \circ Q =$ trace z_0) and consider the operators $\widetilde{z \circ Q} : X \to X$ and $\widetilde{Q \circ z} : X/X_0 \to X/X_0$ (see the diagram (3)). By the principle of related operators [13, 27.3.3], $\operatorname{sp\,tr} \widetilde{z \circ Q} = \operatorname{sp\,tr} \widetilde{Q \circ z}$. By assumption, $\operatorname{sp\,tr} \widetilde{z \circ Q} = \operatorname{trace} z \circ Q$. Now, since X has the AP_α, it follows from the equality trace $z \circ Q =$ trace z_0 that

$$1 = \operatorname{trace} z_0 = \operatorname{sp\,tr} \widetilde{z \circ Q} = \operatorname{sp\,tr} \widetilde{Q \circ z} = \operatorname{sp\,tr} \widetilde{z}_0.$$

Therefore, $\widetilde{z}_0 \neq 0$. By Lemma 4.1, X_0 has the AP_α. The last statement follows from the first part of Proposition 4.2. □

An immediate consequence of Propositions 4.4 and 4.6 is

Proposition 4.7. *Let α be a complete projective tensor quasi-norm of spectral type l_1 such that every Banach space has both the α-extension property and the α-lifting property. If for every $z \in X^* \widehat{\otimes}_\alpha X$ the equality* trace $z =$ sp tr $\widetilde{z}$ *holds, then every quotient of any subspace of X (= every subspace of any quotient of X) possesses the AP_α. Consequently, for $X_0 \subset X_1 \subset X$, $Y = X_1/X_0$ (or for $X_0 \subset X$, $Y \subset X/X_0$) and for every $T \in N_\alpha(Y)$ one has:* trace $T =$ sp tr T.

Proof. Apply in different orders Propositions 4.4 and 4.6. □

4.4. Applications. $\mathbb{Z}_d$-symmetry for $N_{[r,p]}$ and $N^{[r,p]}$

One of our main result (in context of the $\mathbb{Z}_d$-symmetry of the spectra of nuclear operators) is

Theorem 4.1. *Let α be a complete projective tensor quasi-norm of spectral type l_1 and let a Banach space X have the AP_α. For a fixed $d = 2, 3, \dots$, the spectrum of an operator $T \in N_\alpha(X)$ is $\mathbb{Z}_d$-symmetric if and only if* trace $T^{kd+j} = 0$ *for all $k = 0, 1, 2, \dots$ and $j = 1, 2, \dots, d-1$. In particular, if* trace $T \neq 0$, *then $T^2 \neq 0$.*

Proof. Let the spectrum of an operator $T \in N_\alpha(X)$ be $\mathbb{Z}_d$-symmetric. The traces trace T^n $(n \in \mathbb{N})$ are well defined since $T^n \in N_\alpha(X)$ and X has the AP_α. Take an integer $l := kd + j$ with $0 < j < d$. The eigenvalue sequences of T and T^l can be arranged in such a way that $\{\lambda_n(T)^l\} = \{\lambda_n(T^l)\}$ (see [14, 3.2.24, p. 147]). Since the spectrum of T^l is absolutely summable, trace $T^l = \sum_{\lambda \in \mathrm{sp}\,(T^l)} \lambda$, $\sum_{t \in \sqrt[d]{1}} t = 0$ and we may assume that $\{\lambda_m(T^l)\} = \{\lambda_m(T)^l\}$, we get that trace $T^{kd+j} = 0$.

To prove the converse, we need some information from Fredholm Theory. Let u be an element of the projective tensor product $Y^* \widehat{\otimes} Y$, where Y is an arbitrary Banach space. Recall that the Fredholm determinant $\det(1 - wu)$ of u (see [7, Chap. II, §1, $n°4$, p. 13], [6], [13] or [14] is an entire function

$$\det(1 - wu) = 1 - w \text{ trace } u + \cdots + (-1)^n w^n \alpha_n(u) + \cdots,$$

all zeros of which are exactly (according to their multiplicities) the inverses of nonzero eigenvalues of the operator $\widetilde{u}$, associated with the tensor element u. By [7, Chap. II, §1, $n°4$, Corollaire 2, pp. 17–18], this entire function is of the form

$$\det(1 - wu) = e^{-w \text{ trace } u} \prod_{i=1}^{\infty} (1 - ww_i)\, e^{ww_i},$$

where $\{w_i = \lambda_i(\widetilde{u})\}$ is a complete sequence of all eigenvalues of the operator $\widetilde{u}$. Hence, there exists a $\delta > 0$ such that for all w, $|w| \leq \delta$, we have

$$\det(1 - wu) = \exp\Big(\sum_{n=1}^{\infty} c_n\, w^n \text{ trace } u^n\Big) \tag{4}$$

(see [6, p. 350]; cf. [5, Theorem I.3.3, p. 10]).

Now, let trace $T^{kd+r} = 0$ for all $k = 0, 1, 2, \dots$ and $r = 1, 2, \dots, d-1$. By (4), $\det(1 - wT) = \exp\big(\sum_{m=1}^{\infty} c_{md}\, w^{md} \text{ trace } T^{md}\big)$ in a neighborhood V of zero. Hence, for the analytic function $f(w) := \det(1 - wT)$, we have: there exists a $\delta > 0$

such that for all $w, |w| \le \delta$, $f(tw) = f(w)$ for every $t \in \sqrt[d]{1}$. By the uniqueness theorem, the complete system of eigenvalues of T is $\mathbb{Z}_d$-symmetric. □

Applying Theorem 4.1 to the tensor products $\widehat{\otimes}_{[r,p']}$ and $\widehat{\otimes}^{[r,p']}$ and using Example 4.3, we get the following generalizations of Zelikin's theorem:

Theorem 4.2. *Let $0 < r \le 1$, $1 \le p \le 2$, $1/r = 1/2 + 1/p$ and $d = 2, 3, \dots$ For any Banach space X and every operator $T \in N_{[r,p']}(X)$ (or $T \in N^{[r,p']}(Z)$) we have that the spectrum of the operator T is $\mathbb{Z}_d$-symmetric if and only if* trace $T^{kd+j} = 0$ *for all* $k = 0, 1, 2, \dots$ *and* $j = 1, 2, \dots, d-1$. *In particular, if* trace $T \ne 0$, *then* $T^2 \ne 0$.

We obtain Zelikin's theorem, if we put $d = 2$, $r = 1, p = 2$ and $X = H$ (a Hilbert space), since $N_1(H) = S_1(H) = N_{[1,2]}(H) = N^{[1,2]}(H)$.

4.5. Proof of Theorem 1.1

Here it is

Proof. Let $T \in N_r(Y)$. Under the conditions of the theorem we have: every quotient of every subspace of an L_p-space has the AP_r, $\lambda(T) \in l_1$ and the trace of T is well defined and equals the sum of the eigenvalues of T (written in according to their multiplicities; see, e.e., [16, 20]).

Supposing that the spectrum of T is $\mathbb{Z}_d$-symmetric, we can proceed as in the beginning of the proof of Theorem 4.1 to obtain that trace $T^{kd+j} = 0$ for all $k = 0, 1, 2, \dots$ and $j = 1, 2, \dots, d-1$.

To proof the converse, we repeat word for word the second part of the proof of Theorem 4.1. □

4.6. Sharpness of main results

We need the following auxiliary result:

Lemma 4.3. *If $r \in [2/3, 1), q \in (2, \infty]$ and $1/r = 3/2 - 1/q$, then there exist a subspace $Y_q \subset l_q$ (c_0 for $q = \infty$) and a tensor element $w_q \in Y_q^* \widehat{\otimes} Y_q$ so that $w_q \in Y_q^* \widehat{\otimes}^{[s,q]} Y_q$ for every $s > r$,* trace $w_q = 1$ *and $\widetilde{w}_q = 0$. Moreover, w_q can be chosen in such a way that $w_q = \sum_{k=1}^{\infty} e'_k\big|_{Y_q} \otimes y_k$, where (e'_k) is a sequence of the linear functionals on l_q generated by the unit vectors from $l_{q'}$ and (y_k) is in $l_s(Y_q)$ for all $s > r$.*

Proof. Let us look at the proof from [17, Example 2] and take the space Y_q and the tensor element w_q from that proof. We have: Y_q is isometrically imbedded into l_q, $w_q = \sum_{k=1}^{\infty} e'_k\big|_{Y_q} \otimes y_k$, where (e'_k) and (y_k) are as above. □

The following two theorems show that Theorem 4.2 is optimal.

Theorem 4.3. *Let $r \in [2/3, 1)$, $q \in (2, \infty]$, $1/r = 3/2 - 1/q$. There exists a nuclear operator V in l_q (in c_0 for $q = \infty$) such that*

(1) *$V \in N^{[s,q]}(l_q)$ for each $s \in (r, 1]$;*

(2) *V is neither in $N^{[r,q]}(l_q)$ nor r-nuclear;*
(3) trace $V = 1$ *and* $V^2 = 0$.

Proof. Take a pair (Y_q, w_q) from Lemma 4.3 and let $i : Y_q \to l_q$ be an isometric imbedding. Define $v \in l_q^* \widehat{\otimes}\, l_q$ by $v = \sum_{k=1}^{\infty} e'_k \otimes iy_k$ and put $V := \widetilde{v}$. This operator possesses the properties (1)–(3) (we have to mention only that $N^{[r,q]}(l_q) \subset N^r(l_q)$ and that if $T \in N_r(l_q)$ with trace $z = 1$, then $T^2 \neq 0$ by Theorem 1.1). □

Theorem 4.4. *Let $r \in [2/3, 1)$, $p \in [1, 2)$, $1/r = 1/2 + 1/p$. There exists a nuclear operator U in l_p such that*
(1) *$U \in N_{[s,p']}(l_p)$ for each $s \in (r, 1]$;*
(2) *U is neither in $N_{[r,p']}(l_p)$ nor r-nuclear;*
(3) trace $V = 1$ *and* $V^2 = 0$.

Proof. Consider $U := V^*$, where V is from the previous theorem. □

Now, Theorem 1.2 follows from the above theorems, since, e.g., $N^{[s,q]} \subset N^s$.

One more auxiliary fact:

Lemma 4.4. *Let $r \in (2/3, 1], q \in [2, \infty), 1/r = 3/2 - 1/q$. One can find the number sequences (q_k) and (n_k) with $q_n > q, q_n \to q$ and $k_n \to \infty$ for which the following statement is true: There exist a Banach space Y_0 and a tensor element $w \in Y_0^* \widehat{\otimes}_r Y_0$ so that $Y_0 \subset Y := \left(\sum_k l_{q_k}^{n_k}\right)_{l_q}$, $w \neq 0, \tilde{w} = 0$, the space Y_0 (as well as Y_0^*) has the AP_s for every $s < r$ (but does not have the $AP_{r,\bar{q}}$ for any $\bar{q} \in (q, \infty]$). Moreover, w can be chosen in such a way that $w = \sum_{k=1}^{\infty} \sum_{m=1}^{n_k} e'_{mk}\big|_{Y_0} \otimes y_{mk}$, where (e'_{mk}) is a weakly $\bar{q}$-summable $(\forall\, \bar{q} > q)$ sequence of the linear functionals on Y generated by the unit vectors from Y^* and (y_{mk}) is in $l_r(Y_0) \setminus \cup_{s<r} l_s(Y_0)$.*

Proof. It is enough to take the space Y_0 and the tensor element w from the proof of [17, Example 1] and put $n_k := 3 \cdot 2^k$ in that proof. After this we get exactly the desired Banach space and tensor element. We have also: $Y_0 \subset Y \subset l_{\bar{q}}$ for every $\bar{q} > q$. Hence, the sequence $(e'_{mk}\big|_{Y_0})$ is weakly $\bar{q}$-summable $(\forall\, \bar{q} > q)$. □

Theorem 4.5. *Let $r \in (2/3, 1], q \in [2, \infty), 1/r = 3/2 - 1/q$. One can find the number sequences (q_k) and (n_k) with $q_k > q, q_k \to q$ and $n_k \to \infty$ for which the following statement is true:*

There exists a nuclear operator U in $Y := \left(\sum_k l_{q_k}^{n_k}\right)_{l_q}$ such that

(1) *$U \in N^{[r,\bar{q}]}(Y)$ for each $\bar{q} > q$;*
(2) *U is not in $N^{[r,q]}(Y)$;*
(3) trace $U = 1$ *and* $U^2 = 0$.

Proof. Take a pair (Y_0, w) from Lemma 4.4 and let $j : Y_0 \to Y$ be an injection map. Define $u \in Y^* \widehat{\otimes}\, Y$ by $u = \sum_{k=1}^{\infty} \sum_{m=1}^{n_k} e'_{mk} \otimes jy_{mk}$ and put $U := \widetilde{u}$. This operator possesses the properties 1)–3) (we have to mention only that if $T \in N_{[r,q]}(Y)$ with trace $z = 1$, then $T^2 \neq 0$ by Theorem 4.2). □

Theorem 4.6. *Let $r \in (2/3, 1]$, $p \in (1, 2]$, $1/r = 1/2 + 1/p$. One can find the number sequences (p_k) and (n_k) with $p_k < p, p_k \to p$ and $n_k \to \infty$ for which the following statement is true:*

There exists a nuclear operator V in $E := \left(\sum_k l_{p_k}^{n_k}\right)_{l_p}$ such that

(1) *$V \in N_{[r,\bar{q}]}(E)$ for each $\bar{q} > q$;*
(2) *V is not in $N_{[r,q]}(E)$;*
(3) trace $V = 1$ *and* $V^2 = 0$.

Proof. Consider $V := U^*$, where U is from the previous theorem. □

Let us emphasize an important particular case of Theorems 4.5 and 4.6, namely, the case of so-called "asymptotically Hilbertian spaces" (see, e.g., [2] for a definition):

Theorem 4.7. *There exist an asymptotically Hilbertian space $Y_2 := \left(\sum_k l_{q_k}^{n_k}\right)_{l_2}$ ($q_k \to 2$ and $n_k \to \infty$) and a nuclear operator U in this space so that*

1) *$U \in N^{[1,2+\varepsilon]}(Y_2)$ for each $\varepsilon > 0$.*
2) *U is not in $N^{[1,2]}(Y_2)$.*
3) trace $U = 1$ *and* $U^2 = 0$.

The corresponding statements hold for the adjoint operator U^*.

As we know, the last theorem is the best strengthening of related results from [2], [15] and [17].

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A remark on the order of mixed Dirichlet–Neumann eigenvalues of polygons

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Abstract. Given the Laplacian on a planar, convex domain with piecewise linear boundary subject to mixed Dirichlet–Neumann boundary conditions, we provide a sufficient condition for its lowest eigenvalue to dominate the lowest eigenvalue of the Laplacian with the complementary boundary conditions (i.e., with Dirichlet replaced by Neumann and vice versa). The application of this result to triangles gives an affirmative partial answer to a recent conjecture. Moreover, we prove a further observation of similar flavor for right triangles.

1. Introduction

We consider the Laplacian $-\Delta_\Gamma$ on a bounded, convex polygon $\Omega \subset \mathbb{R}^2$ subject to a Dirichlet boundary condition on a part Γ of the boundary and a Neumann boundary condition on the complement Γ^c. The operator $-\Delta_\Gamma$ is self-adjoint and has a purely discrete spectrum, and its lowest eigenvalue λ_1^Γ is positive, provided Γ is nonempty. It is clear that enlarging Γ leads to an increase of λ_1^Γ, but making a different choice of Γ with the same or a larger length may in some cases lead to a smaller value of λ_1^Γ, that is, λ_1^Γ does not depend monotonously on the size of Γ.

The present note provides two observations on monotonicity properties of the lowest eigenvalue with respect to the choice of Γ, and it is inspired by recent results for triangles and other special domains in [8], see also the survey [3]. In the first result of this note, Theorem 3.1, we compare λ_1^Γ to the lowest eigenvalue $\lambda_1^{\Gamma^c}$ of the mixed Laplacian $-\Delta_{\Gamma^c}$ satisfying the complementary boundary conditions, i.e., a Dirichlet condition on Γ^c and a Neumann condition on Γ. We show that the inequality

$$\lambda_1^{\Gamma^c} \leq \lambda_1^\Gamma$$

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holds if Γ^c consists of one single side of the polygon Ω and the two angles where Γ and Γ^c meet are both strictly smaller than $\pi/2$; see Fig. 1 for examples. This

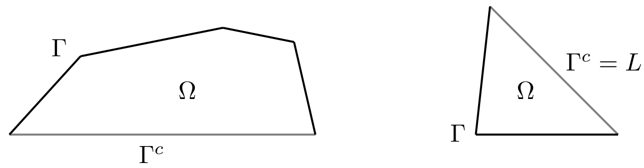

FIGURE 1. Two settings for which $\lambda_1^{\Gamma^c} \leq \lambda_1^{\Gamma}$ holds. In each case, Γ and Γ^c are drawn in black and gray, respectively.

result can be used to affirm a part of a conjecture on the lowest eigenvalues of triangles raised by Siudeja in [8, Conjecture 1.2]. In fact, for an arbitrary triangle whose sides we denote by S, M and L, ordered nondecreasingly by their lengths, it follows

$$\lambda_1^L \leq \lambda_1^{M \cup S},$$

which, to the best of our knowledge, was known before only for certain classes of right triangles.

The second result of this note, Theorem 4.1, is more restrictive and applies only to right triangles. It complements the recent results in [8] by stating that

$$\max\left\{\lambda_1^S, \lambda_1^M\right\} \leq \lambda_1^L$$

holds for any right triangle, i.e., imposing the Dirichlet condition on the hypotenuse always leads to a larger (or equal) lowest eigenvalue than having the Dirichlet condition on one of the catheti.

The proofs of Theorem 3.1 and Theorem 4.1 rely on plugging a certain partial derivative of an eigenfunction into the Rayleigh quotient and using an integral identity for the second partial derivatives of Sobolev functions on polygons. A similar approach was used for the comparison of mixed and Dirichlet Laplacian eigenvalues on polygons and polyhedra in [5], see also [4].

Let us finally mention that properties of eigenvalues of the Laplacian with mixed boundary conditions on special polygons have played an important role in various contexts. For instance, they were used in the famous construction of isospectral domains in [1] and, more recently, in connection with the hot spots conjecture in [7].

2. Preliminaries

Let us set the stage and collect a few ingredients for the proofs of our main results. Recall first that for Γ being any choice of sides of the polygon Ω the (negative)

Laplacian $-\Delta_\Gamma$ can be defined as the self-adjoint operator in $L^2(\Omega)$ which corresponds to the semibounded, closed quadratic form

$$H^1_{0,\Gamma}(\Omega) := \left\{u \in H^1(\Omega) : u\big|_\Gamma = 0\right\} \ni u \mapsto \int_\Omega |\nabla u|^2 \mathrm{d}x.$$

The functions in the domain of $-\Delta_\Gamma$ satisfy a Dirichlet boundary condition on Γ and a Neumann boundary condition (in a weak sense, see, e.g., [6, Lemma 4.3] for a definition of the weak Neumann trace) on the complement $\Gamma^c = \partial\Omega \setminus \Gamma$. If $u \in \operatorname{dom}(-\Delta_\Gamma)$ is sufficiently regular (see Proposition 2.1 below) then the Neumann condition on Γ^c can be interpreted in the usual sense, requiring the trace of $\nabla u \cdot \nu$ to vanish on Γ^c, where ν is the outer unit normal field on the boundary.

The operator $-\Delta_\Gamma$ has a compact resolvent and its lowest eigenvalue λ_1^Γ is positive provided Γ is nonempty. It is nondegenerate and can be expressed by the variational identity

$$\lambda_1^\Gamma = \min_{u \in H^1_{0,\Gamma}(\Omega)} \frac{\int_\Omega |\nabla u|^2 \mathrm{d}x}{\int_\Omega |u|^2 \mathrm{d}x}. \tag{2.1}$$

Below we make use of the following regularity result which follows from [2, Theorem 4.4.3.3 and Lemma 4.4.1.4].

Proposition 2.1. *Assume that all angles at which Γ and Γ^c meet are strictly less than $\pi/2$. Then* $\operatorname{dom}(-\Delta_\Gamma) \subset H^2(\Omega)$.

Moreover, we will significantly make use of the following identity, which is a consequence of [2, Lemma 4.3.1.1–4.3.1.3].

Lemma 2.2. *Let $u \in H^2(\Omega)$ satisfy a Dirichlet boundary condition on Γ and a Neumann boundary condition on its complement Γ^c. Then*

$$\int_\Omega (\partial_{12} u)^2 \mathrm{d}x = \int_\Omega (\partial_{11} u)(\partial_{22} u) \mathrm{d}x.$$

We emphasize that the latter statement is valid for polygons only and fails for more general, curved domains.

3. An ordering result for the lowest mixed eigenvalues of polygons

In this section we prove the following first result of this note.

Theorem 3.1. *Let $\Omega \subset \mathbb{R}^2$ be a polygon and suppose $\Gamma \subset \partial\Omega$ is such that $\Gamma^c = \partial\Omega \setminus \Gamma$ consists of one single line segment. Moreover, suppose that the angles at both vertices where Γ and Γ^c meet are strictly less than $\pi/2$. Then*

$$\lambda_1^{\Gamma^c} \leq \lambda_1^\Gamma.$$

Proof. Without loss of generality we assume that Γ^c is parallel to the x_2-axis. Let u be a real-valued eigenfunction of $-\Delta_\Gamma$ corresponding to the eigenvalue λ_1^Γ, and let $v = \partial_1 u$. It follows from Proposition 2.1 that v belongs to $H^1(\Omega)$. Moreover, since u satisfies a Neumann boundary condition on Γ^c and the first unit vector $(1,0)^\top$ is normal to Γ^c, it follows $v\big|_{\Gamma^c} = 0$, i.e., v is an admissible test function for the Rayleigh quotient of $-\Delta_{\Gamma^c}$. Note that v is nontrivial since $\partial_1 u = 0$ identically on Ω together with $u\big|_\Gamma = 0$ would imply $u = 0$ on Ω. We employ Lemma 2.2 to obtain

$$\begin{aligned}
0 &= \int_\Omega \big((\partial_{11}u)(\partial_{22}u) - (\partial_{12}u)^2\big)\mathrm{d}x = \int_\Omega \big((\partial_{11}u)\Delta u - (\partial_{11}u)^2 - (\partial_{12}u)^2\big)\mathrm{d}x \\
&= -\lambda_1^\Gamma \int_\Omega \operatorname{div}\begin{pmatrix}\partial_1 u\\ 0\end{pmatrix} u\mathrm{d}x - \int_\Omega \big((\partial_{11}u)^2 + (\partial_{12}u)^2\big)\mathrm{d}x \\
&= \lambda_1^\Gamma \Big(\int_\Omega \begin{pmatrix}\partial_1 u\\ 0\end{pmatrix}\cdot \nabla u\mathrm{d}x - \int_{\partial\Omega} u\begin{pmatrix}\partial_1 u\\ 0\end{pmatrix}\cdot \nu\mathrm{d}\sigma\Big) - \int_\Omega |\nabla(\partial_1 u)|^2\mathrm{d}x \\
&= \lambda_1^\Gamma \int_\Omega (\partial_1 u)^2\mathrm{d}x - \int_\Omega |\nabla(\partial_1 u)|^2\mathrm{d}x,
\end{aligned} \tag{3.1}$$

where in the last step we have used $u|_\Gamma = 0$ and $\partial_1 u\big|_{\Gamma^c} = 0$. It follows

$$\int_\Omega |\nabla v|^2\mathrm{d}x = \lambda_1^\Gamma \int_\Omega v^2\mathrm{d}x, \tag{3.2}$$

and the assertion of the theorem follows with the help of the identity (2.1) applied to Γ^c instead of Γ. □

Remark 3.2. The idea of using derivatives of eigenfunctions as test functions was used in [4] to establish eigenvalue inequalities between Dirichlet and Neumann eigenvalues of the Laplacian on smooth domains. In [5] it was used to compare mixed and Dirichlet eigenvalues on polygons and polyhedra. We remark that the methods of [5] may be employed to extend Theorem 3.1 to higher dimensions.

Next we apply Theorem 3.1 to triangles and obtain the following three statements. If Ω is a triangle we denote its sides by S, M and L, in nondecreasing order of their lengths. We remark that the inequality (iii) in the following corollary is a part of Conjecture 1.2 in [8].

Corollary 3.3. *If Ω is any triangle then the following assertions hold:*

(i) *If both angles enclosing S are strictly less than $\pi/2$ then $\lambda_1^S \le \lambda_1^{L\cup M}$.*
(ii) *If both angles enclosing M are strictly less than $\pi/2$ then $\lambda_1^M \le \lambda_1^{L\cup S}$.*
(iii) *In any case, $\lambda_1^L \le \lambda_1^{M\cup S}$.*

Proof. The assertions (i) and (ii) are direct consequences of Theorem 3.1. For item (iii) just note that the angles enclosing the longest edge of a triangle can never be equal to or larger than $\pi/2$. □

4. A remark on the lowest eigenvalues of right triangles

In this short section we restrict ourselves to the class of right triangles and compare the lowest eigenvalue for a Dirichlet condition on a cathetus to the one for the hypotenuse, see Fig. 2. This extends observations from [8, Theorem 1.1] (where additional restrictions on the angles were required) to right triangles with arbitrary angles.

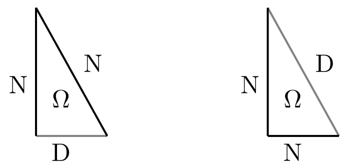

FIGURE 2. Two choices of mixed boundary conditions on the same right triangle (D = Dirichlet, N = Neumann). By Theorem 4.1 the lowest eigenvalue of the left configuration does not exceed the lowest eigenvalue of the right one.

Theorem 4.1. *Let Ω be a right triangle with sides S, M and L ordered nondecreasingly by their lengths. Then*

$$\max\left\{\lambda_1^S, \lambda_1^M\right\} \leq \lambda_1^L.$$

Proof. We show the inequality $\lambda_1^S \leq \lambda_1^L$; the inequality $\lambda_1^M \leq \lambda_1^L$ is analogous. The proof is similar to the proof of Theorem 3.1. Let us assume w.l.o.g. that S is parallel to the x_2-axis. We take a nontrivial, real-valued $u \in \ker\left(-\Delta_L - \lambda_1^L\right)$ and set $v = \partial_1 u$. Then v is nontrivial and $v|_S = 0$. Now we repeat the calculation (3.1) with $\Gamma = L$ and observe that the boundary integral is zero since u vanishes on L, which is the hypotenuse, $\partial_1 u$ vanishes on S, and for the other cathetus, M, the normal vector ν is plus or minus the second unit vector $(0,1)^\top$. Hence we arrive at (3.2) with $\Gamma = L$, which completes the proof. □

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Linear Operators and Operator Functions Associated with Spectral Boundary Value Problems

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Dedicated to the memory of Boris Pavlov (1936–2016)

Abstract. The paper develops a theory of spectral boundary value problems from the perspective of general theory of linear operators in Hilbert spaces. An abstract form of spectral boundary value problem with generalized boundary conditions is suggested and results on its solvability complemented by representations of weak and strong solutions are obtained. Existence of a closed linear operator defined by a given boundary condition and description of its domain are studied in detail. These questions are addressed on the basis of Krein's resolvent formula derived from the explicit representations of solutions also obtained here. Usual resolvent identities for two operators associated with two different boundary conditions are written in terms of the so called M-function. Abstract considerations are complemented by illustrative examples taken from the theory of partial differential operators. Other applications to boundary value problems of analysis and mathematical physics are outlined.

Keywords. Spectral boundary value problem, singular perturbations, Krein's resolvent formula, linear operators, M-function, open systems theory.

1. Introduction

Close relationships between studies of boundary value problems and the linear operator theory are well known to specialists in both disciplines.

As an example, one can only mention numerous attempts to translate properties of solutions to boundary value problems into the operator-theoretic language that culminated in the development of an important branch of contemporary mathematics, the interpolation theory of linear operators and scales of Banach and Hilbert spaces [10, 45, 49]. Another achievement of the abstract operator theory

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in relation to boundary problems arising in applications is the extension theory of symmetric operators. With its origin in quantum mechanics and operating in the setting of Hilbert spaces, the extension theory suggests a convenient model of boundary value problems rooted in Hilbert space operator theory [2]. Although the abstract approach often turns out to be too generic and therefore additional considerations are required to complete the study, the extension theory of symmetric operators continues to be an important and widely used tool in the studies of boundary value problems in abstract settings. During past decades it was substantially enhanced and enriched by various applications to the operator theory itself, to the classical and functional analysis, and to the mathematical physics. The long list of publications [7, 9, 11, 14, 15, 17, 18, 21, 22, 23, 24, 25, 26, 29, 30, 31, 35, 37, 38, 42, 43, 48, 52, 53, 54, 55, 64, 65, 66, 67, 68, 85] reflects only a small portion of the sheer amount of ongoing studies in the field of extensions theory of symmetric operators.

The present paper offers an operator-theoretic treatment of boundary value problems. The main topic under discussion is the existence of Hilbert space operators corresponding to abstract linear boundary value problems defined by suitably generalized boundary conditions. As is well known, many applications of the partial differential equations theory entail problem statements characterized by certain types of formally written boundary conditions. In the case of second order partial differential equations on bounded or unbounded domains such conditions are usually rendered in terms of linear combinations of boundary values of solutions and traces of their derivatives evaluated on the domain boundary. Typical examples include the Laplacian in a domain of Euclidian space with Dirichlet, Neuman, or Robin boundary conditions. Depending on the nature of these conditions, the resulting problem may or may not give rise to a closed linear operator in a Hilbert or Banach space. If such an associated operator exists, then the study is effectively reduced to the analysis of its properties. The paper describes a wide class of boundary conditions that determine a closed linear operator in a Hilbert space and studies its spectral characteristics in the general setting.

In a sense, the goal pursued here is opposite to the treatment by G. Grubb [35] where the existence of boundary conditions corresponding to a given closed realization of an elliptic operator is investigated.

An essential part of present research is the formulation of generic linear boundary value problems in the language of Hilbert space operator theory. Within this framework, boundary conditions are defined by two parameters, two closed linear operators acting in the "boundary space." Reiteration of the material developed earlier in [71, 73] is followed by a more detailed inquiry into the properties of solutions, which in turn leads to Krein's resolvent formula and usual resolvent identities for closed operators acting on the "main space" corresponding to various boundary conditions. Spectral properties of these operators are described in terms of the so called M-function.[1] Several examples offered throughout the text illustrate the main ideas.

The ongoing study of M-functions, also known as m-, Q-, Weyl–Titchmarsh functions, Steklov–Poincaré operator, Dirichlet-to-Neumann maps, transfer functions, etc., forms a significant part of the contemporary boundary value problems studies. The M-functions theory originates in the concept of the m-function for singular Sturm–Liouville differential equations [83]. Since then the notion of M-functions has been generalized to other settings and followed by deep results on M-function properties and applications. We only mention a few relevant papers concerning topics in scattering theory [63, 84], Schrödinger and Sturm–Liouville operators theory [8], inverse problems [39, 80], the spectral asymptotic [27, 75], extensions of symmetric operators and adjoint pairs [14, 15, 17, 21, 22, 23, 24, 25, 48, 53, 54, 55], numerous studies on partial differential operators including operators in non-smooth domains [7, 28, 29, 30, 31, 32, 33], the numerical spectral analysis [16, 56], singular perturbations [64, 65, 66], and the linear systems theory [71, 73]. In the present paper's context M-functions are realized as operator-functions with values in the set of closed linear operators acting in the "boundary space," a Hilbert space associated with the "boundary."

Operator theoretic parts of the present work have some overlaps with the extensions theory of linear symmetric operators and relations in Hilbert and Krein spaces based on the notion of so called boundary triplets [18, 42] and their generalizations. This approach relies on the properties of the abstract Green's formula that involves a linear symmetric operator (a linear symmetric relation in general case) and two linear boundary maps into the "boundary space." The theory of boundary triplets is one of the most generic treatments of general boundary relations available today. The interested reader is referred to the original papers [21, 22, 23, 24, 25, 26, 52, 53, 54, 55] where further references can be found. Another successful approach to the extension theory of symmetric operators was elaborated by A. Posilicano in works [64, 65, 66, 67, 68]. It is rooted in a close relationship between singular perturbations of elliptic differential operators and the extensions theory [4, 5]. In comparison with these studies, the present study follows the line of reasoning found in [71, 73]. The ideas expounded below are inspired by the Birman–Krein–Vishik method of extensions of positive operators in Hilbert space [11, 44, 85] (see also [35, 37, 6]), the Weyl decomposition [86], the open systems theory [51], and the theory of linear systems with boundary control [77]. As a result, the framework in this paper is not centered around symmetric operators and does not involve any notions specific to the extensions theory. It is built from the first principles concerning linear operators and their domains, as well as properties of linear sets in Hilbert spaces. The linear systems theory conveniently provides an adequate language to communicate the underpinnings

[1] Values of all M-functions under consideration are closed linear operators acting in Hilbert spaces, with one exception of the example given in Sect. 7 where M-function is a matrix function. Sometimes the term "M-operators" is used in order to stress the operator theoretic nature of M-function [8].

of this approach. With some risk of oversimplification, the last part of Sect. 2 explains these ideas in more depth by connecting them to the objects of systems theory. The paper's treatment of boundary value problems from the abstract point of view opens a possibility to consider classical and non-classical applications from a uniform perspective. As an example, it turns out that obtained results offer a straightforward interpretation of boundary value problems when the "boundary" does not exist a priori and has to be constructed artificially. This type of problems has been well studied in the literature and is usually referred to as singular perturbations of differential operators characterized by perturbations supported on the sets of Lebesque measure zero (often called the null sets). The well known quantum mechanical model of point interactions [4, 5] and the study of more general Schrödinger operators with potentials supported by null sets [3] are typical examples. This fact underlines close connections of the present material to the papers [64, 65, 66, 67, 68] devoted to the study of extensions of symmetric operators and singular perturbations. In the field of linear systems theory singular perturbations represent the procedure of "channels opening" connecting an initially closed systems to its environment [51]. From this point of view, the M-function is naturally identified with the transfer function of the resulting open system interacting with its environment by means of these channels. Operator theoretic treatment also illuminates ideas behind the so-called "Dirichlet decoupling" [20] also known as "Glazman's splitting procedure" [34] and establishes connections to the analog of Weyl–Titchmarsh function of multidimensional Schrödinger operator [8, 73]. It appears relevant to other problems of mathematical physics, e.g., the exterior complex scaling in the theory of resonances [76] and the R-matrix method well known in nuclear physics [47]. Some of these applications are discussed in Sect. 7 and in the last part of Sect. 2 where relevant bibliographical references can be found; these ideas are the topics of further research.

The approach to spectral boundary value problems adopted in the paper has certain limitations. One of them is the assumption of selfadjointness and bounded invertibility of the "main" operator (denoted A_0 throughout) acting in the Hilbert space H. The requirement of bounded invertibility of A_0 can be weakened to the condition $\mathrm{Ker}(A_0 + cI) = \{0\}$ for some $c \in \mathbb{R}$, but the selfadjointess is essential. Nevertheless, the schema can be extended to the case $A_0 \neq A_0^*$, but only at the expense of introducing the so called dual pairs [53, 54, 55] (see also [14, 15, 17]), which makes the study much more involved. Another limitation is the preference to work with linear operators, rather than with linear relations (multivalued operators) which appears to be the recent trend in the literature, see especially [22, 23]. The language of single valued operators stands more in line with the classical approach of operator theory and is preferred here. One more requirement is that the operator A_0 must be unbounded so that the range of A_0^{-1} is dense in H. Fortunately, all these restrictions do not impede the study of the main question addressed in the paper, that is, the description of operators corresponding to boundary value problems defined in terms of boundary conditions.

Let us now briefly overview the paper's structure. Section 2 offers an accessible introduction into the setting of boundary problems and M-functions. It serves as a guideline for the topics discussed later and provides a concise exposition of the operator theoretic framework of spectral boundary value problems independent of the symmetric operators theory. The main example is the well known spectral problem for Dirichlet Laplacian in a smooth domain in $\mathbb{R}^n$, $n \geq 3$. An adequate language for study of this operator is the language of Green's functions, integral equations and layer potentials. When necessary, relevant results are freely borrowed from the standard references [1, 57, 58]. By this example all essential ingredients of the following exposition are explicitly formulated and finally compiled in a short catalog. Relationships to the extension theory of symmetric operators, Krein's resolvent formula, and resolvent identities are also discussed. Since the linear systems theory plays an important role for the approach employed in this work, a brief explanation of the principal ideas of this theory is provided for reader's convenience. At the end of section other cases of partial differential operators that can be treated in a similar fashion are mentioned.

Section 3 develops the machinery required for the purposes of the paper. The main objective here is to formulate notions useful for the study of spectral boundary value problems and associated M-functions given in terms of their basic underlying objects. Such objects are two Hilbert spaces and three closed linear operators satisfying certain compatibility conditions. The solvability theorem is proven and ensuing definitions of weak and strong solutions are discussed. The section concludes with alternative descriptions of M-functions and some comments regarding their properties.

Spectral boundary value problems with general boundary conditions are investigated in Sect. 4. After the problem statement the solvability theorem is proven and expressions for the solutions corresponding to various boundary conditions are obtained. The last part of the section explores a general definition of M-functions associated with two different boundary conditions.

Section 5 is the main contribution of the paper. We discuss the existence of closed linear operators corresponding to spectral boundary value problems and subsequent study of their properties. Formal expressions for the resolvents and parameters of "boundary conditions" are derived from the general representation of solutions obtained in the previous section. These expressions are rigorously justified alongside with the study of spectral properties of respective operators and detailed descriptions of their domains. Relations to the extension theory of symmetric operators are also explained. The section closes with a brief digression into the original Birman–Krein–Vishik theory [11, 44, 85] and remarks on its connections to the present study.

Section 6 offers a sketch of scattering theory for operators associated with boundary value problems. Simultaneously, by virtue of the paper's approach, all arguments of this section remain valid for singular perturbations of partial differential operators by "potentials" concentrated on null sets. Form the operator-theoretic point of view, the primary interest here is the link between the boundary value problems theory and the functional model of nonselfadjoint operators established by means of Cayley transform applied to the M-function. It is shown that the ideas of papers [60, 61] devoted to the functional model based approach to the scattering theory are easily adopted and are fully applicable for the comprehensive development of scattering theory of linear boundary value problems, selfadjoint and nonselfadjoint alike. Section 6 can be seen as a groundwork for the future study in this direction.

The last section is an illustration of the boundary value problem technique discussed in the paper in application to singular perturbations of multidimensional differential operators. A simple example of the quantum mechanical model for a finite number of point interactions in $L^2(\mathbb{R}^3)$ (see [4, 5]) is studied. A familiar interpretation in the form of Schrödinger operator with δ-potentials is given and additional comments regarding singular perturbations concentrated on the null sets are supplied. Reported results are by no means new; most of them can be easily found in the relevant literature cited in the text. The objective of this section is to demonstrate how the abstract schema presented in earlier chapters can be put to practice for the study of particular cases of multidimensional differential operators.

Notation. Symbols $\mathbb{R}$, $\mathbb{C}$, $\operatorname{Im}(z)$ stand for the real axis, the complex plane, and the imaginary part of a complex number $z \in \mathbb{C}$, respectively. The upper and lower half planes are the open sets $\mathbb{C}_\pm := \{z \in \mathbb{C} \mid \pm \operatorname{Im}(z) > 0\}$. If A is a linear operator on a separable Hilbert space H, the domain, range and null set of A are denoted $\mathcal{D}(A)$, $\mathcal{R}(A)$, and $\operatorname{Ker}(A)$, respectively. For two separable Hilbert spaces H_1 and H_2 the notation $A : H_1 \to H_2$ is used for a bounded linear operator A defined everywhere in H_1 with the range in the space H_2. The symbol $\rho(A)$ is used for the resolvent set of A. For a Hilbert space H the term *subspace* always denotes a closed linear set in H. The closure of operators and sets is denoted by the horizonal bar over the corresponding symbol. All Hilbert spaces are assumed separable.

2. Boundary Value Problems by Example

In this introductory section we recall the classical example of the boundary value problem and M-function associated with the Dirichlet Laplacian in a simply connected bounded domain with smooth boundary in the Euclidian space. The purpose of this exposition is twofold. First, it reminds the reader of the concept of M-functions, and secondly it brings together facts that serve as a foundation for the general approach developed further. The *italic typeface* is used to highlight those observations which are essential for the investigations of the present paper. Results cited below hold true under much weaker assumptions, e.g., for elliptic differential operators on non-smooth domains including Lipschitz subdomains of Riemannian manifolds, see [41, 58, 59] and references therein. For further details the reader is referred to many expositions of the boundary integral equations method in application to boundary value problems for elliptic equations and systems, see [1, 57, 58] for relevant references.

Dirichlet problem. Let $\Omega \subset \mathbb{R}^n$, $n \geq 3$ be a bounded simply connected domain with $C^{1,1}$-boundary Γ. The Laplace differential expression $\Delta = \sum_i \frac{\partial^2}{\partial x_i^2}$ defined on smooth functions in Ω generates the Dirichlet Laplacian Δ_D in $L^2(\Omega)$. The domain of $A_0 := -\Delta_D$ consists of functions from the Sobolev class $H^2(\Omega)$ with null traces on Γ. *The operator A_0 is selfadjoint and boundedly invertible in $L^2(\Omega)$.*

Harmonic functions and operator of harmonic continuation. Let γ_0 be the trace operator that maps continuous functions u defined in the closure $\overline{\Omega}$ of Ω into their traces on the boundary, $\gamma_0 : u \mapsto u|_\Gamma$. *It follows from the definition of $-\Delta_D$ that* $\gamma_0 A_0^{-1} = 0$. For $\varphi \in C(\Gamma)$ denote h_φ the solution of the Dirichlet problem in Ω:

$$\Delta u = 0, \qquad \gamma_0 u = \varphi, \quad \text{where } \varphi \in C(\Gamma)$$

The operator $\Pi : \varphi \mapsto h_\varphi$ is bounded as a mapping from $L^2(\Gamma)$ into $L^2(\Omega)$ and $\mathrm{Ker}(\Pi) = \{0\}$, see [58]. It is readily seen that Π is the classical operator of harmonic continuation from the boundary Γ into the domain Ω uniquely extended to the bounded linear map defined on the space $L^2(\Gamma)$. The equality $\gamma_0 \Pi \varphi = \varphi$ continues to hold for $\varphi \in L^2(\Gamma)$ and moreover $\Delta h_\varphi = 0$ for $h_\varphi = \Pi\varphi$ in the sense of distributions [58]. Observe that the (unbounded and not closed) operator A : $A_0^{-1} f \dot{+} \Pi\varphi \mapsto f$, $f \in L^2(\Omega)$, $\varphi \in L^2(\Gamma)$ is well defined since *the domain of operator A_0 and the set $\mathcal{R}(\Pi)$ do not have nontrivial common elements*, otherwise A_0 would not be boundedly invertible:

$$\exists\, A_0^{-1} \Longrightarrow \mathcal{D}(A_0) \cap \mathcal{R}(\Pi) = \{0\}.$$

The same argument shows that $\mathcal{D}(A_0)$ does not contain any nontrivial functions from $H^2(\Omega)$ satisfying the homogenous equation $(-\Delta - zI)h = 0$ under the assumption $z \in \rho(A_0)$. Obviously, A_0 is a restriction of A to $\mathcal{D}(A_0)$. Notice also that A does not coincide with the "maximal operator" defined as an adjoint to the map $u \mapsto -\Delta u$, where $u \in L^2(\Omega)$ belongs to the class C_0^∞ of infinitely differentiable functions vanishing in the vicinity of boundary Γ.

Adjoint of the harmonic continuation operator. Let $G(x, y)$ be the Green's function of $A_0 = -\Delta_D$, so that $(A_0^{-1} f)(x) = \int_\Omega G(x, y) f(y)\, dx$ for $f \in L^2(\Omega)$, see [58]. The kernel $G(\cdot, \cdot)$ is symmetric and real-valued: $G(x, y) = G(y, x)$ and $\overline{G(x, y)} = G(x, y)$. Denote by $d\sigma$ the normalized Lebesgue surface measure on Γ. Then the operator Π can be expressed as an integral operator with Poisson kernel

$$\Pi : \varphi \mapsto -\int_\Gamma \varphi(y) \frac{\partial}{\partial \nu_y} G(x, y)\, d\sigma_y$$

where $\frac{\partial}{\partial \nu}$ is the derivative along the outside pointing normal at the boundary Γ. For a smooth function f in Ω

$$(\Pi\varphi, f) = -\int_\Omega \left(\int_\Gamma \varphi(y) \frac{\partial}{\partial \nu_y} G(x, y)\, d\sigma_y \right) \overline{f(x)}\, dx,$$

and due to Fubini's theorem and properties of $G(\cdot,\cdot)$,

$$(\Pi\varphi, f) = -\int_\Gamma \varphi(y)\,\frac{\partial}{\partial\nu_y}\left(\int_\Omega \overline{f(x)}\;G(x,y)\,dx\right)d\sigma_y$$
$$= -\left\langle \varphi, \frac{\partial}{\partial\nu}\left(\int_\Omega G(x,\cdot)\,f(x)\,dx\right)\right\rangle$$

where $\langle\cdot,\cdot\rangle$ denotes the inner product in $L^2(\Gamma)$. Since $G(x,y) = G(y,x)$ is the integral kernel of A_0^{-1}, we obtain *the representation for* Π^**, the adjoint of* Π,

$$\Pi^* = \gamma_1 A_0^{-1}$$

where $\gamma_1 : u \mapsto -\gamma_0\frac{\partial u}{\partial\nu} = -\left.\frac{\partial u}{\partial\nu}\right|_\Gamma$. We will use the symbol ∂_ν for the map $u \mapsto \left.\frac{\partial u}{\partial\nu}\right|_\Gamma$, so that $\gamma_1 = -\partial_\nu$.

The spectral problem. The spectral Dirichlet boundary value problem for the differential expression $\Delta = \sum_i \frac{\partial^2}{\partial x_i^2}$ in Ω is defined by the system of equations for $u \in \mathcal{D}(A) := \mathcal{D}(A_0)\dot{+}\mathcal{R}(\Pi)$, namely

$$\begin{cases}(A - zI)u = 0,\\ \gamma_0 u = \varphi\end{cases} \tag{2.1}$$

where $A : u \mapsto -\Delta u$, $\varphi \in L^2(\Gamma)$, and the number $z \in \mathbb{C}$ plays the role of spectral parameter. For $z \in \rho(A_0)$ the distributional solution u_z^φ can be obtained from the harmonic function $\Pi\varphi$ by the formula $u_z^\varphi = (I - zA_0^{-1})^{-1}\Pi\varphi$. Indeed, since $(I - zA_0^{-1})^{-1} = I + z(A_0 - zI)^{-1}$ and $A\Pi\varphi = 0$ in the distributional sense, we have

$$(A - zI)u_z^\varphi = (A - zI)\left(\Pi\varphi + z(A_0 - zI)^{-1}\Pi\varphi\right) = -z\Pi\varphi + z\Pi\varphi = 0,$$

due to the identity $(A - zI)(A_0 - zI)^{-1} = I$. Therefore the vector u_z^φ is a solution to the equation $(A - zI)u = 0$. Further, $\gamma_0 u_z^\varphi = \gamma_0\Pi\varphi = \varphi$. Hence *the vector* $u_z^\varphi = (I - zA_0^{-1})\Pi\varphi$ *is a solution to the spectral problem* (2.1) *for* $\varphi \in L^2(\Gamma)$ *and* $z \in \rho(A_0)$.

Solution Operator and DN-Map. For the spectral problem (2.1) with $\varphi \in L^2(\Gamma)$ and $z \in \rho(A_0)$ introduce the solution operator

$$S_z : \varphi \mapsto (I - zA_0^{-1})^{-1}\Pi\varphi \tag{2.2}$$

Operator S_z is bounded as a mapping from $L^2(\Gamma)$ into $L^2(\Omega)$. For $\varphi \in C^2(\Gamma)$ the inclusion $S_z\varphi \in H^2(\Omega)$ holds and therefore the expression $\gamma_1 S_z\varphi$ is well defined. The operator function $M(z)$ defined by

$$M(z) : \varphi \mapsto \gamma_1 S_z\varphi, \quad \varphi \in C^2(\Omega) \tag{2.3}$$

is analytic in $z \in \rho(A_0)$. It is called the Dirichlet-to-Neumann map (DN-map) or, more generally, the M-function of $A = -\Delta$ in the domain Ω. By construction, $-\partial_\nu u = M(z)\,(u|_\Gamma)$ for $u \in \mathrm{Ker}(A - zI)$ as long as the function $\gamma_0 u = u|_\Gamma$ is sufficiently smooth on Γ. In fact, it can be shown that values of so defined $M(z)$, $z \in \rho(A_0)$ are closed operators acting in $L^2(\Gamma)$ with the domain $H^1(\Gamma)$, see [81] and references therein.

The representation $S_z = (I - zA_0^{-1})^{-1}\Pi$ and equality $\Pi^* = \gamma_1 A_0^{-1}$ imply

$$(S_z)^* = \gamma_1 A_0^{-1}(I - \bar{z}A_0^{-1})^{-1} = \gamma_1(A_0 - \bar{z}I)^{-1}. \tag{2.4}$$

Therefore $S_z = [\gamma_1(A_0 - \bar{z}I)^{-1}]^*$ and the M-function $M(z)$ can be rewritten as

$$M(z) = \gamma_1[\gamma_1(A_0 - \bar{z}I)^{-1}]^*.$$

In particular, $M(0) = \gamma_1(\gamma_1 A_0^{-1})^* = \gamma_1\Pi$. It can be shown (see [81]) that *the operator $M(0) = \gamma_1\Pi$ defined on the domain $\mathcal{D}(M(0)) = H^1(\Gamma)$ is selfadjoint in* $L^2(\Gamma)$. Operator $M(0)$ turns out to be a rather important object; it is convenient to use a special notation for it:

$$\Lambda = M(0) = \gamma_1\Pi, \quad \mathcal{D}(\Lambda) = H^1(\Gamma).$$

Robin Boundary Conditions. Let $\beta \in L^\infty(\Gamma)$ be a bounded function defined almost everywhere on the boundary Γ. In what follows we also denote β the bounded operator of multiplication $\varphi \mapsto \beta\varphi$, $\varphi \in L_2(\Gamma)$ acting in the space $L_2(\Gamma)$. Consider the boundary value problem

$$\begin{cases} (A - zI)u = 0, \\ -\partial_\nu u + \beta u|_\Gamma = \varphi \end{cases} \tag{2.5}$$

with $\varphi \in L^2(\Gamma)$. In particular, for $\beta = 0$ we recover the classical Neumann problem for the Laplacian in Ω. For nontrivial β the system (2.5) is called the boundary problem of third type, or Robin problem. Assume $z \in \rho(A_0)$ and let u_z^φ be a smooth solution to the first equation, that is $(A - zI)u_z^\varphi = 0$. Because $\gamma_1 u_z^\varphi = M(z)\gamma_0 u_z^\varphi$, the second equation for the trace $\psi := \gamma_0 u_z^\varphi$ becomes $(\beta + M(z))\psi = \varphi$. Suppose the map $(\beta + M(z))$ is boundedly invertible as an operator in $L^2(\Gamma)$. Then the boundary equation for ψ can be solved explicitly: $\psi = (\beta + M(z))^{-1}\varphi$. In turn, the solution u_z^φ is recovered from its trace $\psi = \gamma_0 u_z^\varphi$ by the mapping S_z:

$$u_z^\varphi = (I - zA_0^{-1})^{-1}\Pi\gamma_0 u_z^\varphi = (I - zA_0^{-1})^{-1}\Pi(\beta + M(z))^{-1}\varphi, \tag{2.6}$$

where $z \in \rho(A_0)$ is such that $(\beta + M(z))^{-1}$ exists. Observe that application of γ_1 to both sides of this equality yields the expression for the map $\varphi \mapsto \gamma_1 u_z^\varphi$, which by analogy with the DN-map can be called the Robin-to-Neumann map:

$$M_{RN}(z) = M(z)(\beta + M(z))^{-1}.$$

Similarly, application of γ_0 yields an expression for the Robin-to-Dirichlet map:

$$M_{RD}(z) = (\beta + M(z))^{-1}. \tag{2.7}$$

Krein's resolvent formula and Hilbert resolvent identity. Equations (2.5) give rise to another boundary problem, namely the problem for an unknown function u in Ω satisfying

$$\begin{cases} (A - zI)u = f, \\ \gamma_1 u + \beta\gamma_0 u = 0 \end{cases} \tag{2.8}$$

with $f \in L^2(\Omega)$, where $\gamma_1 u = -\partial_\nu u = -\frac{\partial u}{\partial \nu}|_\Gamma$ and $\gamma_0 u = u|_\Gamma$. It is customary to look for a solution to (2.8) in the form

$$u_z^f = (A_0 - zI)^{-1} f + S_z \psi = (A_0 - zI)^{-1} f + (I - zA_0^{-1})^{-1} \Pi \psi \tag{2.9}$$

with $z \in \rho(A_0)$ and some $\psi \in L^2(\Gamma)$ to be determined. Since $(A - zI)(A_0 - zI)^{-1} f = f$ and $(A - zI) S_z \psi = 0$, the first equation (2.8) is satisfied by (2.9) automatically; therefore we only need to find $\psi \in L^2(\Gamma)$ such that (2.9) obeys the boundary condition in (2.8). Applying γ_0 and γ_1 to (2.9) we obtain

$$\begin{aligned} \gamma_0 u_z^f &= \gamma_0 S_z \psi = \psi, \\ \gamma_1 u_z^f &= \gamma_1 (A_0 - zI)^{-1} f + \gamma_1 S_z \psi = \Pi^* (I - zA_0^{-1})^{-1} f + M(z)\psi. \end{aligned}$$

Now the relation $\Pi^* = \gamma_1 A_0^{-1}$, properties of solution operator S_z and the definition of $M(z)$, lead to the following equation for the unknown function ψ

$$0 = (\gamma_1 + \beta\gamma_0) u_z^f = \Pi^* (I - zA_0^{-1})^{-1} f + (\beta + M(z))\psi.$$

Again, assuming $z \in \rho(A_0)$ is such that $(\beta + M(z))$ is boundedly invertible, the formula for ψ follows:

$$\psi = -(\beta + M(z))^{-1} \Pi^* (I - zA_0^{-1})^{-1} f.$$

Substitution into (2.9) yields the result

$$u_z^f = (A_0 - zI)^{-1} f - (I - zA_0^{-1})^{-1} \Pi (\beta + M(z))^{-1} \Pi^* (I - zA_0^{-1})^{-1} f. \tag{2.10}$$

This expression certainly requires some justification as the second summand need not be smooth and thereby the normal derivative $-\partial_\nu u_z^f$ that appears in the boundary condition may be undefined for some $f \in L^2(\Omega)$. But let us defer discussion of this difficulty to the main body of the paper and turn instead to the operator-theoretic interpretation of the equations (2.8) and their solution (2.10).

The system (2.8) represents a problem of finding a vector u from the domain of operator $\mathcal{A}_\beta$ defined as a restriction of A to the set of functions $u \in L^2(\Omega)$ satisfying the boundary condition $(\gamma_1 + \beta\gamma_0)u = 0$ in some yet undefined sense. It is clear that $\mathcal{A}_\beta$ also can be treated as an extension of the so-called *minimal operator* defined as $A = -\Delta$ restricted to the set $C_0^\infty(\Omega)$ of infinitely differentiable functions in Ω that vanish in some neighborhood of Γ along with all their partial derivatives. Assuming for the sake of argument that each vector $u \in \mathcal{D}(\mathcal{A}_\beta)$ satisfies the condition $(\gamma_1 + \beta\gamma_0)u = 0$ literally, that is the expression $(\gamma_1 + \beta\gamma_0)u$ makes sense for each $u \in \mathcal{D}(\mathcal{A}_\beta)$, the problem (2.8) with $f \in L^2(\Omega)$ is the familiar resolvent equation $(\mathcal{A}_\beta - zI)u = f$ for the operator $\mathcal{A}_\beta$. Therefore the solution (2.10) for $z \in \rho(\mathcal{A}_\beta)$ coincides with $(\mathcal{A}_\beta - zI)^{-1} f$. We see that the resolvents of A_0 and $\mathcal{A}_\beta$ for $z \in \rho(A_0) \cap \rho(\mathcal{A}_\beta)$ are related by the following identity commonly known as *Krein's resolvent formula*

$$(\mathcal{A}_\beta - zI)^{-1} = (A_0 - zI)^{-1} - (I - zA_0^{-1})^{-1} \Pi (\beta + M(z))^{-1} \Pi^* (I - zA_0^{-1})^{-1}. \tag{2.11}$$

Notice that the right-hand side of (2.11), depends on $(\beta + M(z))^{-1}$ which is exactly the M-function (2.7). Under assumption of bounded invertibility of $\beta + M(0)$ in

$L^2(\Gamma)$ we have

$$\mathcal{A}_\beta^{-1} = A_0^{-1} - \Pi(\beta + M(0))^{-1}\Pi^*. \tag{2.12}$$

This expression shows in particular that while the difference of $\mathcal{A}_\beta$ and A_0 is only defined *a priori* on the set of smooth functions u vanishing on the boundary Γ along with their first derivatives where $(\mathcal{A}_\beta - A_0)u = 0$, the difference of their inverses $\mathcal{A}_\beta^{-1} - A_0^{-1}$ is a nontrivial bounded operator in $L^2(\Omega)$. As a consequence, if $\beta = \beta^*$, then the operator $\mathcal{A}_\beta$ is selfadjoint as an inverse of a sum of two bounded selfadjoint operators. Moreover, the formula (2.12) can be successfully employed for the investigation into spectral properties of $\mathcal{A}_\beta$, as it reduces the boundary problem setting to the well-developed case of perturbation theory for bounded operators (cf. [35]).

Krein's formula (2.11) implies another useful identity relating resolvents of A_0 and $\mathcal{A}_\beta$ to each other. According to the definition of solution operator S_z the identity $\gamma_0(I - zA_0^{-1})^{-1}\Pi = I$ holds for any $z \in \rho(A_0)$. Hence, application of γ_0 to both sides of (2.11) leads to

$$\gamma_0(\mathcal{A}_\beta - zI)^{-1} = (\beta + M(z))^{-1}\Pi^*(I - zA_0^{-1})^{-1}. \tag{2.13}$$

Krein's formula can now be rewritten in the form

$$(\mathcal{A}_\beta - zI)^{-1} - (A_0 - zI)^{-1} = -(I - zA_0^{-1})^{-1}\Pi\gamma_0(\mathcal{A}_\beta - zI)^{-1}.$$

By substituting the adjoint of $S_z = (I - zA_0^{-1})^{-1}\Pi$ from (2.4) we obtain the following variant of *Hilbert resolvent identity* for A_0 and $\mathcal{A}_\beta$ (cf. [30, 31])

$$(A_0 - zI)^{-1} - (\mathcal{A}_\beta - zI)^{-1} = [\gamma_1(A_0 - \bar{z}I)^{-1}]^*\gamma_0(\mathcal{A}_\beta - zI)^{-1}, \quad z \in \rho(A_0) \cap \rho(\mathcal{A}_\beta). \tag{2.14}$$

Finally, notice that all considerations above are valid at least formally if the symbol β in the condition (2.8) represents a linear bounded operator acting on the Hilbert space $L^2(\Gamma)$.

Summary. Observations of this section lay down a foundation for the study of boundary value problems and M-functions presented in the paper. For further convenience, this preliminary discussion concludes by summing up properties of operators A_0 and Π and their relationships to the boundary maps γ_0, γ_1 that are relevant for our study.

- Operator A_0^{-1} is bounded, selfadjoint, and $\operatorname{Ker}(A_0^{-1}) = \{0\}$.
- Operator Π is bounded and $\operatorname{Ker}(\Pi) = \{0\}$.
- The intersection $\mathcal{D}(A_0) \cap \mathcal{R}(\Pi) = \mathcal{R}(A_0^{-1}) \cap \mathcal{R}(\Pi)$ is trivial.
- The left inverse of Π is the trace operator γ_0 restricted to $\mathcal{R}(\Pi)$, that is $\gamma_0\Pi\varphi = \varphi$ for $\varphi \in L^2(\Gamma)$.
- The set $\mathcal{D}(A_0) = \mathcal{R}(A_0^{-1})$ is included into the null space of γ_0, so that $\gamma_0 A_0^{-1} = 0$.
- The adjoint operator of Π is expressed in terms of γ_1 and A_0 as $\Pi^* = \gamma_1 A_0^{-1}$.
- Operator $\Lambda = \gamma_1\Pi$ is selfadjoint (and unbounded) in $L^2(\Gamma)$.

Further, the spectral boundary value problem $(A - zI)u = 0$, $\gamma_0 u = \varphi$, where A is an extension of A_0 to the set $\mathcal{D}(A_0)\dot{+}\mathcal{R}(\Pi)$ defined as $Ah = 0$ for $h \in \mathcal{R}(\Pi)$, gives rise to the solution operator S_z and to the M-function $M(z)$, $z \in \rho(A_0)$.

- The solution operator has the form $S_z = (I - zA_0^{-1})^{-1}\Pi$, $z \in \rho(A_0)$.
- The M-function is formally defined by the equality $M(z) = \gamma_1 S_z$, $z \in \rho(A_0)$.

Finally, the boundary condition associated with the expression $\gamma_1 + \beta\gamma_0$ where β is a linear operator in $L^2(\Gamma)$ defines the Robin boundary value problem and the corresponding linear operator $\mathcal{A}_\beta$.

- The resolvents of $\mathcal{A}_\beta$ of A_0 are related by Krein's formula (2.11) expressed in terms of M-function (2.7).
- Hilbert resolvent identity (2.14) holds.

The linear systems theory perspective. As stated in Introduction, ideas underlying the operator theoretic framework employed for the paper's purpose are partially inspired by the approach to boundary value problems found in the linear systems theory. These ideas are best illustrated by considering the following variant of problem (2.1)

$$\begin{cases} Au = f, \\ \gamma_0 u = \varphi \end{cases} \tag{2.15}$$

where all participating objects are as in (2.1) and the vector f is an arbitrary function from $L^2(\Omega)$. From the point of view of linear systems theory, equations (2.15) describe a linear system with the state space $H = L^2(\Omega)$, the input-output space $E = L^2(\Gamma)$ and the main operator A. Solutions to (2.15) are called "internal states" of the system and vectors $\varphi \in L^2(\Gamma)$ are interpreted as the system's input. The system's output is defined by the operator γ_1 that maps internal states of the system to elements of the input-output space E.

When the input in (2.15) is absent ($\varphi = 0$), the corresponding internal state is obviously $u^f = A_0^{-1}f$. This situation corresponds to the closed system, that is, the system that is isolated from the external influences modeled by inputs $\varphi \in E$. The closed system still has a nontrivial output given by $\gamma_1 : u^f \mapsto \gamma_1 A_0^{-1} f = \Pi^* f$. Introduction of the non-zero input $\varphi \in E$ in (2.15) is a way to open the system to external influences. As can be easily verified, the procedure of system opening results in an additional term in the expression for the state vectors, $u^{f,\varphi} = A_0^{-1}f + \Pi\varphi$. The output of the system defined by the operator γ_1 results in the mapping from internal states to outputs in the form $\gamma_1 : u^{f,\varphi} \mapsto \gamma_1 A_0^{-1} f + \gamma_1\Pi\varphi$. At this point we need to take into consideration the unboundedness of the trace operator γ_1 and only choose inputs resulting in the outputs that belong to $E = L^2(\Gamma)$. All such inputs (admissible inputs) therefore are functions $\varphi \in L^2(\Gamma)$ for which the harmonic continuations $\Pi\varphi$ into the domain Ω possess normal derivatives with traces on Γ from the space $L^2(\Gamma)$. With an appropriate choice of inputs $\varphi \in L^2(\Gamma)$, the system's output is determined by the map $\gamma_1 : u^{f,\varphi} \mapsto \Pi^* f + \Lambda\varphi$, where we employed notation $\Lambda = \gamma_1\Pi$ introduced earlier and used the equality $\gamma_1 A_0^{-1} = \Pi^*$.

The restriction of admissible inputs to a smaller set in this example is dictated by the choice of output operator γ_1 that cannot be defined on all attainable internal states $\{u^{f,\varphi} \mid f \in H, \varphi \in E\}$ of the system. Such a restriction, however, does not create any inconvenience. Quite the opposite, this feature can be perceived as an advantage of the approach, because it allows for the definition of inputs according to the particular problem at hand.[2] Note also that an alternative approach consists of suitable alterations of outputs that do not change essential properties of the system under investigation, and at the same time widen the set of admissible inputs (see [15, 17] in this regard for an example of "regularization procedure" applied to the system's output).

The internal states of the linear system described by equations (2.15) are therefore represented as the sum of two components, $u^{f,\varphi} = A_0^{-1} f + \Pi\varphi$. The first term is always a function from the domain of Dirichlet Laplacian, and the second term needs not be smooth and belong to the domain of $A = -\Delta$ at all. It is a function from the range of the operator of harmonic continuation from the boundary, $\Pi : L^2(\Gamma) \to L^2(\Omega)$. These two components are linearly independent in the sense of equivalence $\{u^{f,\varphi} = 0\} \iff \{A_0^{-1} f = 0, \Pi\varphi = 0\}$. In other words, the internal states of the system are vectors from the direct sum $\mathcal{D}(A_0) \dot{+} \mathcal{R}(\Pi)$. In the language of linear systems theory the second summand is associated with the set of controls imposed on the system. The equality $\operatorname{Ker}(\Pi) = \{0\}$ means that this set stands in a one-to-one correspondence with the set of all inputs. Operator Π that maps inputs into controls is often called the *control operator*.

For the "spectral" case of linear system described by equations (2.1) the system's input are again vectors $\varphi \in L^2(\Gamma)$ and the internal state is determined by the solution operator $\varphi \mapsto S_z\varphi$ for $z \in \rho(A_0)$, see (2.2). Following the systems theory language, if the output is defined by means of operator γ_1 as $\gamma_1 S_z\varphi$, then the M-function (2.3) is nothing but the transfer function of this system that maps the input φ into the output $\gamma_1 S_z\varphi$ (for suitable $\varphi \in E$). The resolvent identity and formula $\Pi^* = \gamma_1 A_0^{-1}$ allow to rewrite (2.3) as

$$M(z) = \Lambda + z\Pi^*(I - zA_0^{-1})^{-1}\Pi, \quad z \in \rho(A_0). \tag{2.16}$$

This representation has important consequences.

First, the function (2.16) is expressed in terms of three linear operators, A_0^{-1}, Π, and Λ, playing very specific and well defined roles in the description of linear system corresponding to (2.1). Namely, many applications of the systems theory interpret the spectral parameter $z \in \mathbb{C}$ in (2.1) as the frequency of oscillations taking place inside Ω. Typical and well known examples are classical acoustic and electromagnetic waves existing in the domain Ω. The operator $\Lambda = M(0)$ then has the meaning of system's response at zero frequency, and can be interpreted as the operator of static reaction. Since its independence on the spectral parameter it

[2]This situation is common in practical applications of the systems theory where the set of inputs is always subject to the real world limitations. For instance, it is clear that only smooth functions from $L^2(\Gamma)$ can be realized in practice as the system's inputs. Therefore the ability to choose input vectors freely conforms to the standard assumptions of systems theory.

maps inputs directly to the outputs without applying any z-dependent (therefore, frequency dependent) transformations. In the systems theory terms the operator Λ is usually called the *feedthrough operator*. Consequently, with a given input $\varphi \in E$ the second term in (2.16) describes oscillations of the system around its "static reaction" $\Lambda\varphi$. Notice that for $z \in \rho(A_0)$ the second term is a bounded operator in E. Also of interest is the observation that the feedthrough operator Λ is independent of operators A_0 and Π describing oscillations, and therefore can be chosen to suit specific requirements of the given application.[3]

Secondly, as described above, the operator of harmonic continuation $\Pi : L^2(\Gamma) \to L^2(\Omega)$ translates inputs into controls. Its adjoint Π^* is called the *observation operator* because according to (2.16) it maps internal states $S_z\varphi = (I - zA_0^{-1})^{-1}\Pi\varphi$ into the system's output, thereby making internal states available to the external observer. The equality $\Pi^* = \gamma_1 A_0^{-1}$ is crucial for the representation (2.16) of M-operator initially defined as $M(z) = \gamma_1 S_z$. For the model example of the Laplacian discussed above the identity $\Pi^* = \gamma_1 A_0^{-1}$ is a consequence of Fubini's theorem and properties of Green's function. To ensure validity of the representation (2.16) within the general framework, the definition of abstract counterpart of γ_1 given below explicitly involves operator Π^*, see Definition 3.3.

Finally, from the theoretical point of view the system is considered a "black box," with the transfer function being the only source of information about its internals available to the observer. It follows that the linear system defined by equations (2.1) or (2.15) with the internal states-outputs map γ_1 is completely described by the operators A_0^{-1}, Π, and Λ participating in the representation (2.16) of its transfer function. In other words, the study of (2.1) from the systems theory perspective is equivalent to the study of the set $\{A_0^{-1}, \Pi, \Lambda\}$.

The transition from the system defined in terms of $\{A, \gamma_0, \gamma_1\}$ to the system defined by $\{A_0^{-1}, \Pi, \Lambda\}$ is known in the systems theory as *reciprocal transform*, see [19, 77, 73]. These two systems share the state and input–output spaces, their transfer functions coincide, but their defining operators are different. One advantage of the reciprocal transform is that it translates operators $\{A, \gamma_0, \gamma_1\}$ that are often difficult to describe in practical applications into the set of well defined and closed operators $\{A_0^{-1}, \Pi, \Lambda\}$, two of which are bounded. For instance, the Laplacian $A = -\Delta$ in the domain Ω from the model example above, when defined in its "natural domain," that is, the Sobolev space $H^2(\Omega)$, is not a closed operator in $L^2(\Omega)$. At the same time the mappings γ_0 and γ_1 are well defined on $H^2(\Omega)$, although they are not closed on their domains either. The procedure of operator theoretic closure of $A = -\Delta$ in the space $L^2(\Omega)$ results in the operator $\overline{A} = clos(-\Delta)$ with the domain that contains elements from $L^2(\Omega) \setminus H^2(\Omega)$. Because the null set of a closed operator is always closed, $\mathcal{D}(\overline{A})$ contains at least the L^2-closure

[3]See publications [15, 17] as an example, where the authors modify the system's output by subtracting the static reaction, thereby working with the system with the output defined as $(\gamma_1 - \Lambda\gamma_0)u^\varphi$ and consequently with the null feedthrough operator. Here $\varphi \in E$ is the input and $u^\varphi \in H$ is the corresponding internal state.

of all harmonic functions continuous in $\overline{\Omega}$. This set includes functions that need not to possess boundary values on Γ, so that the boundary mappings γ_0, γ_1 can not be defined on all elements from $\mathcal{D}(\overline{A})$. Therefore the choice of suitable domain for A and subsequent expressions for boundary operators are not always obvious (except for the simplest cases, involving a boundary space of finite dimensionality as one example). In contrast, operators of the reciprocal system $\{A_0^{-1}, \Pi, \Lambda\}$ are all well defined and always closed. They are the solution operator of the Dirichlet problem in the domain Ω, the operator of harmonic continuation from the boundary Γ into Ω, and the classical Dirichlet-to-Neumann map for the Laplacian in Ω, respectively.

References to the reciprocal transform also help to clarify the relationship between the paper's framework and the mentioned earlier approach based on the notion of boundary triples. The starting point for the latter is the set $\{\overline{A}, \gamma_0, \gamma_1\}$ (where $\overline{A}$ is the operator-theoretic closure of A) that gives rise to an abstract Green's formula, as opposed to the discussion below carried out on the basis of operators $\{A_0^{-1}, \Pi, \Lambda\}$ that define the "reciprocal" system. In order to circumvent the described above difficulties with the operator domains the earlier versions of boundary triples approach [24, 25, 26] severely limited its applicability by requesting the operator A to be closed, γ_0, γ_1 to be bounded in the graph norm of A, and the ranges of γ_0, γ_1 to coincide with the boundary space E. The last assumption is the most restrictive, as it automatically excludes from consideration unbounded M-functions. These limitations were removed only recently, see papers [9, 22], opening further possibilities of non trivial applications to the partial differential operators. In contrast, the approach based on the set $\{A_0^{-1}, \Pi, \Lambda\}$ offers a framework free of these restrictions. It not only allows one to work with closed and bounded operators, but also gives an option to selectively choose inputs from the boundary space E, thus eliminating the concern of a suitable domain definition for boundary mappings and removing the assumption of closedness (and even closability) of A. It is also worth mentioning that when operators $\{\overline{A}, \gamma_0, \gamma_1\}$ form a "boundary triplet," all three of them are mutually interdependent. Their domains must be suitably chosen and their definitions must fit together in order for the Green's formula to hold. In the "reciprocal" approach, only two operators, A_0 and Π, are interdependent (the intersection of their ranges must be trivial), whereas the operator Λ (both its action and its domain) can be selected arbitrarily. Qualitatively speaking, one may say that the boundary triples method goes "from the inside to the outside" relating elements of the state space H to elements in the boundary space E by means of operators γ_0 and γ_1, whereas the approach adopted in this paper goes in the opposite direction by introducing the control operator Π that maps elements from the boundary space into elements of the state space. Operator Λ then, as a feedthrough operator acting on the boundary space, is an arbitrary parameter that does not have to be closed and even closable.

Applications. Translation of classic boundary value problems and their solution procedures to the operator theoretic language suggests applicability of the obtained results in various settings. As one example, it seems rather natural to consider a more general type of boundary conditions (2.8) written as $(\alpha\gamma_1 + \beta\gamma_0)u = 0$ with some linear operators α, β acting on $L^2(\Omega)$ (or even bounded operator valued functions $\alpha(z)$, $\beta(z)$ of the spectral parameter $z \in \mathbb{C}$). If $\beta = \chi_E$ is the characteristic function of a non empty measurable set $E \subset \Gamma$ of positive Lebesgue surface measure on Γ and $\alpha = 1 - \chi_E$, then the boundary condition above takes the form $(1 - \chi_E)\partial_\nu u + \chi_E u|_\Gamma = 0$. It describes the so called mixed boundary value problem (Zaremba's problem) with the Dirichlet boundary condition on E and the Neumann condition on $\Gamma \setminus E$ (cf. [58]).

The abstract operator theoretic technique elaborated in the paper can be successfully applied to the study of boundary value problems of classic and modern complex analysis. In particular, it is possible to reformulate within the abstract framework classic problems of Poincaré, Hilbert, and Riemann for harmonic and analytic functions in bounded simply connected and sufficiently smooth domains of the complex plane, see [74]. The generic boundary conditions in the form $(\alpha\gamma_1 + \beta\gamma_0)u = 0$ appear rather naturally in these cases.

One more example is based on the earlier study [73] and is discussed here at some length. Using the above notation, it concerns the transmission type boundary condition imposed on solutions to the equation $(-\Delta - \zeta I)u = 0$ inside and outside of Ω. It is convenient to rewrite this equation as $(A - zI)u = 0$ with $A = -\Delta + I$ and $z = \zeta + 1$ for reasons that will be clarified shortly. Denote $u_z^\pm$ its solutions in the domains $\Omega^\pm$ where $\Omega^- = \Omega$ and $\Omega^+ = \mathbb{R}^n \setminus \overline{\Omega}$. Then the boundary condition $(\partial_\nu u_z^-)|_\Gamma - (\partial_\nu u_z^+)|_\Gamma = \varphi$ with $\varphi \in L^2(\Gamma)$ defines a variant of transmission problem. Here $(\partial_\nu u_z^\pm)|_\Gamma$ are boundary values on Γ of the normal derivatives of functions $u_z^\pm$ in the direction of outer normal to the domain Ω. The solution to this problem is given by the single layer potential

$$(\mathscr{S}_z\varphi)(x) := \int_\Gamma G(x, y, z)\varphi(y)d\sigma_y, \quad x \in \mathbb{R}^n$$

where $G(\cdot, \cdot, z)$ is the standard Green's function of the differential operator $(-\Delta + I - zI)$ and $d\sigma_y$ is the Euclidian surface measure on Γ. In order to include this problem into the paper's framework, define operators γ_0 and γ_1 acting on linear combinations of smooth functions $v^\pm \in L^2(\Omega^\pm)$ with the property $v^-|_\Gamma = v^+|_\Gamma = v|_\Gamma \in C(\Gamma)$ as maps

$$\gamma_0 : v \mapsto (\partial_\nu v^-)|_\Gamma - (\partial_\nu v^+)|_\Gamma, \quad \gamma_1 : v \mapsto v|_\Gamma$$

where we put $v := v^+ + v^- \in L^2(\mathbb{R}^n)$. Properties of single layer potentials are such that boundary values on Γ of the function $\mathscr{S}_z\varphi$ taken from Ω^+ and Ω^- coincide almost everywhere. Moreover, the difference of boundary values of normal derivatives of $\mathscr{S}_z\varphi$ from inside and outside of Ω are equal to φ almost everywhere. In other words, $\gamma_0\mathscr{S}_z\varphi$ and $\gamma_1\mathscr{S}_z\varphi$ are well defined and $\gamma_0\mathscr{S}_z\varphi = \varphi$. Now it is only a matter of interpretation to treat this transmission problem as a spectral problem in the form (2.1). The solution operator S_z obviously coincides with $\varphi \mapsto \mathscr{S}_z\varphi$ and the choice of operator γ_1 made above leads to the M-function being the single layer potential restricted to Γ, that is, $M(z)\varphi = \mathscr{S}_z\varphi|_\Gamma$. Corresponding expressions for Π and $M(0) = \gamma_1\Pi$ easily follow from their definitions. More precisely, since $\Pi = \mathscr{S}_z|_{z=0}$ we have $\Pi\varphi = \mathscr{S}_0\varphi$ and $M(0)\varphi = \mathscr{S}_0\varphi|_\Gamma$.

The expression for $A_0 = A|_{\mathrm{Ker}(\gamma_0)}$ deserves further discussion. Since A is initially defined on the domain of all functions $v \in L^2(\mathbb{R}^n)$, smooth in $\Omega^\pm$ and continuous in $\mathbb{R}^n$, the condition $\gamma_0 v = 0$ makes A_0 equal to $-\Delta + I$ defined on the domain of standard Laplacian $-\Delta$ in $L^2(\mathbb{R}^n)$ (after the conventional operator closure procedure). This fact follows from the embedding theorems for Sobolev classes H^2, according to which the function $v = v^- + v^+$, where $v^\pm \in H^2(\Omega^\pm)$ belongs to $H^2(\mathbb{R}^n)$ if $v^-|_\Gamma = v^+|_\Gamma$ and $(\partial_\nu v^-)|_\Gamma = (\partial_\nu v^+)|_\Gamma$ almost everywhere on Γ. Also note that the addition of identity operator I to the Laplacian $-\Delta$ ensures bounded invertibility of A_0. Operator defined by (2.8) with $\beta = 0$ (that is, by the condition $\gamma_1 u = 0$) is the orthogonal sum of two Dirichlet Laplacians acting in $L^2(\Omega^-) \oplus L^2(\Omega^+)$. A more general transmission problem corresponding to the boundary condition $\alpha(v|_\Gamma) + \beta[(\partial_\nu v^-)|_\Gamma - (\partial_\nu v^+)|_\Gamma] = \varphi$ with $\varphi \in L^2(\Gamma)$ and bounded operators α, β acting in $E = L^2(\Gamma)$ is a particular case of problems investigated in the present paper.

It is also clear that the setting of transmission problem can be interpreted as a case of singular perturbations of quantum mechanics [3, 4, 5], where the "free" Laplacian defined initially in all space $\mathbb{R}^n$ is perturbed by the "potential" supported by the surface Γ. Various boundary conditions in the form $(\alpha\gamma_0 + \beta\gamma_1)u = 0$ with γ_0, γ_1 as above and suitable choice of linear operators α, β acting in $L^2(\Gamma)$ reflect the variety of possible "parameterizations" available in this model. Another illustration of the point of view based on the theory of singular perturbations is given in the last section.

Naturally, the same considerations are applicable to more generic elliptic differential operators in place of the Laplacian, as long as the single layer potential constructed by the Green's function of such operators possesses the same boundary properties as the conventional "acoustic" potential $\mathscr{S}_z$, see [1, 57, 58]. In particular, the Schrödinger operator $-\Delta + q(x)$ in $L^2(\mathbb{R}^n)$ with sufficiently regular real valued function $q(x)$ satisfies this condition. It is a remarkable fact that when $n = 3$, $q \in L^\infty(\mathbb{R}^3)$ and $\Omega = \{x \in \mathbb{R}^3 \mid |x| < 1\}$ the M-function defined by the theory elaborated in the paper coincides with the Weyl–Titchmarsh function of the three-dimensional Schrödinger operator obtained in [8] by the multidimensional analogue of the classical nesting procedure of the Sturm–Liouville theory [83] (see [73] for the proof). Thus the single layer potential constructed by the Green's function of Schrödinger operator with the density supported by the unit sphere in $\mathbb{R}^3$ is a direct multidimensional equivalent of the celebrated Weyl-Titchmarsh m-function.

A similarly developed theory for double layer potentials results in another type of transmission boundary conditions; the M-function in this case coincides with the (unbounded) hypersingular integral operator acting in $L^2(\Gamma)$. The "unperturbed" operator A_0 then is the "free" Laplacian acting in $L^2(\mathbb{R}^n)$, whereas the operator defined by the condition $\gamma_1 u = 0$ is the orthogonal sum of two Neumann

Laplacians acting in $L^2(\Omega^-) \oplus L^2(\Omega^+)$. The interested reader is referred to the publication [73] for proofs and further details.

3. Spectral Boundary Value Problem and its M-function

This section is concerned with a framework used in the study of spectral boundary value problems conducted in Sects. 5 and 6. A substantial part of the material covered here is an exposition of certain facts that can be found in the literature. For the most general perspective, the reader is referred to the works [21, 22, 23] and references therein carried out in a very generic setting of abstract boundary relations. In fact, principal results communicated here can be derived from the exhaustive treatment of [22] as a particular case. Remark 3.6 at the end of section outlines a possible approach for such a derivation and also clarifies existing relationships between [22] and the setting of present paper. The main goal of this section is to give a concise account of all relevant facts in the form convenient for the present study alongside with adequate proofs. Topics covered include the definition of spectral boundary value problem complemented by a discussion of properties of its solutions and the definition of corresponding M-function. An abstract analogue of the operator γ_1 from Sect. 2 leading to the Green's formula and to the concept of weak solutions is elaborated in some depth. The study is conducted under the following assumption.

Let H, E be two separable Hilbert spaces, A_0 be a linear operator in H defined on the dense domain $\mathcal{D}(A_0)$ in H and let $\Pi : E \to H$ be a bounded linear mapping.

Assumption 1. *Suppose the following:*

- *Operator A_0 is selfadjoint and boundedly invertible in H.*
- *Mapping Π possesses the left inverse $\widetilde{\Gamma}_0$ defined on $\mathcal{R}(\Pi)$ by $\widetilde{\Gamma}_0 : \Pi\varphi \mapsto \varphi$, $\varphi \in E$.*
- *The intersection of $\mathcal{D}(A_0)$ and $\mathcal{R}(\Pi)$ is trivial, $\mathcal{D}(A_0) \cap \mathcal{R}(\Pi) = \{0\}$.*

Remark 3.1. As shown in [22], conditions of Assumption 1 can be substantially weakened. In particular, boundary mappings Γ_0 and Γ_1 in the context of [22] are multivalued operators *(*linear relations*)* defined on the graph of operator A that need not be single-valued, nor have a dense domain *(*compare with the definitions of Γ_0, Γ_1, and A in our case below*)*. In addition, bounded invertibility of A_0 is not required for validity of a number of statements found in this section.

Under Assumption 1 neither of sets $\mathcal{D}(A_0)$ and $\mathcal{R}(\Pi)$ coincides with the whole space H. In follows that A_0 is necessarily unbounded. Furthermore, existence of the left inverse of Π implies $\mathrm{Ker}(\Pi) = \{0\}$. The condition $\mathcal{D}(A_0) \cap \mathcal{R}(\Pi) = \{0\}$ is essential. It guarantees existence of (unbounded) projections from the direct sum $\mathcal{D}(A_0) \dot{+} \mathcal{R}(\Pi)$ into the each component parallel to another. In turn, it ensures correctness of definitions of operators A and Γ_0 in the next paragraph. Finally, note that for a non-invertible selfadjoint operator A_0 with a real regular point $c \in$

$\rho(A_0) \cap \mathbb{R}$ the invertibility condition can be easily satisfied by considering the operator $A_0 - cI$ in place of A_0.

Introduce two linear operators A and Γ_0 on the domain $\mathcal{D}(A) = \mathcal{D}(\Gamma_0) \subset H$ by

$$\mathcal{D}(A) := \mathcal{D}(A_0)\dot{+}\mathcal{R}(\Pi) = \{A_0^{-1}f + \Pi\varphi \,|\, f \in H, \varphi \in E\}, \tag{3.1}$$

$$A : A_0^{-1}f + \Pi\varphi \mapsto f, \quad \Gamma_0 : A_0^{-1}f + \Pi\varphi \mapsto \varphi, \quad f \in H, \varphi \in E. \tag{3.2}$$

Operators A and Γ_0 are extensions of A_0 and $\widetilde{\Gamma}_0$ to $\mathcal{D}(A)$ defined to be the null mapping on the complementary subsets $\mathcal{R}(\Pi)$ and $\mathcal{D}(A_0)$, respectively. Observe that $\mathrm{Ker}(A) = \mathcal{R}(\Pi)$ and $\mathrm{Ker}(\Gamma_0) = \mathcal{R}(A_0^{-1})$ $(= \mathcal{D}(A_0))$ since $\mathrm{Ker}(A|_{\mathcal{D}(A_0)})$ and $\mathrm{Ker}(\Gamma_0|_{\mathcal{R}(\Pi)})$ are trivial by construction.

Definition 3.1. *Spectral boundary problem associated with the pair A_0, $\widetilde{\Gamma}_0$ satisfying Assumption 1 consists of the system of linear equations for an unknown element $u \in \mathcal{D}(A)$*

$$\begin{cases} (A - zI)u = f, \\ \Gamma_0 u = \varphi, \end{cases} \qquad f \in H, \varphi \in E, \tag{3.3}$$

where $z \in \mathbb{C}$ is the spectral parameter.

Theorem 3.1. *For $z \in \rho(A_0)$ and any $f \in H$, $\varphi \in E$ there exists a unique solution $u_z^{f,\varphi}$ to the problem* (3.3) *given by the formula*

$$u_z^{f,\varphi} = (A_0 - zI)^{-1}f + (I - zA_0^{-1})^{-1}\Pi\varphi. \tag{3.4}$$

Moreover, if for some $f \in H$ and $\varphi \in E$ the vector defined by the right-hand side of (3.4) *is null, then $f = 0$ and $\varphi = 0$.*

Proof. We will show that the first term in (3.4) is a solution to the system (3.3) with $\varphi = 0$, $f \neq 0$ and the second one solves the system (3.3) for $f = 0$, $\varphi \neq 0$. To that end let us verify first that $(I - zA_0^{-1})^{-1}\Pi\varphi$ belongs to $\mathrm{Ker}(A - zI)$. We have

$$\begin{aligned}(A - zI)(I - zA_0^{-1})^{-1}\Pi\varphi &= (A - zI)\left(I + z(A_0 - zI)^{-1}\right)\Pi\varphi \\ &= \left(A - zI + z(A - zI)(A_0 - zI)^{-1}\right)\Pi\varphi \\ &= (A - zI + zI)\,\Pi\varphi = A\Pi\varphi \\ &= 0\end{aligned}$$

since $A_0 \subset A$ and $\mathrm{Ker}(A) = \mathcal{R}(\Pi)$. Therefore

$$(A - zI)u_z^{f,\varphi} = (A - zI)(A_0 - zI)^{-1}f = f.$$

For the second equation (3.3) and $u_z^{f,\varphi}$ as in (3.4) ,

$$\Gamma_0 u_z^{f,\varphi} = \Gamma_0(I - zA_0^{-1})^{-1}\Pi\varphi = \Gamma_0(I + z(A_0 - zI)^{-1})\Pi\varphi = \Gamma_0\Pi\varphi = \varphi$$

because $\mathrm{Ker}(\Gamma_0) = \mathcal{D}(A_0) = \mathcal{R}((A_0 - zI)^{-1})$. Both equations (3.3) are therefore satisfied.

Uniqueness of the solution (3.4) is a direct consequence of assumption $z \in \rho(A_0)$. For $z = 0$ the implication $u_0^{f,\varphi} = 0 \Longrightarrow f = 0, \varphi = 0$ trivially holds due to uniqueness of the decomposition $u_0^{f,\varphi} = A_0^{-1} f + \Pi\varphi$ into the sum of two terms from disjoint sets and equalities $\mathrm{Ker}(A_0^{-1}) = \{0\}$, $\mathrm{Ker}(\Pi) = \{0\}$. For $z \in \rho(A_0)$ with the help of identity $(I - zA_0^{-1})^{-1} = I + z(A_0 - zI)^{-1}$ the representation (3.4) can be rewritten as

$$u_z^{f,\varphi} = (A_0 - zI)^{-1}(f + z\Pi\varphi) + \Pi\varphi.$$

The first summand here belongs to $\mathcal{D}(A_0)$ and the second to $\mathcal{R}(\Pi)$. Since the intersection of these two sets is trivial, the equality $u_z^{f,\varphi} = 0$ implies $\Pi\varphi = 0$ and thus $\varphi = 0$. Then $(A_0 - zI)^{-1} f = 0$ and therefore $f = 0$. □

Definition 3.2. *Assuming $z \in \rho(A_0)$ denote $R_z = (A_0 - zI)^{-1}$ the resolvent of A_0 and introduce the solution operator $S_z : E \to E$*

$$S_z : \varphi \mapsto (I - zA_0^{-1})^{-1}\Pi\varphi = (I + zR_z)\Pi\varphi, \quad \varphi \in E,\ z \in \rho(A_0).$$

Remark 3.2. An alternative name for the solution operator commonly accepted in the theory of linear symmetric operators and relations is *γ-field*, see [21, 22, 23] and references therein. The present paper follows the terminology inherited from the theory of boundary value problems [37] in order to stress out the role mapping S_z plays in the considerations below.

Remark 3.3. Important properties of the solution operator follow from its definition and the resolvent identity (see [22, Proposition 4.11] for the general case). Suppose $z \in \rho(A_0)$. Then $\Gamma_0 S_z = I$ and $\mathcal{R}(S_z) = \mathrm{Ker}(A - zI)$. Moreover,

$$S_z - S_\zeta = (z - \zeta) R_z S_\zeta, \quad z, \zeta \in \rho(A_0). \tag{3.5}$$

Proof. The first claim follows from Theorem 3.1. The same theorem shows that the range of S_z is included into $\mathrm{Ker}(A - zI)$. To show that $\mathcal{R}(S_z) = \mathrm{Ker}(A - zI)$ assume $u = A_0^{-1} f + \Pi\varphi$ with $f \in H$, $\varphi \in E$ is such that $u \in \mathrm{Ker}(A - zI)$. Then

$$0 = (A - zI)u = (A - zI)(A_0^{-1} f + \Pi\varphi) = (I - zA_0^{-1}) f - z\Pi\varphi$$

so that $f = z(I - zA_0^{-1})^{-1}\Pi\varphi$. Substitution into $u = A_0^{-1} f + \Pi\varphi$ gives

$$u = A_0^{-1} f + \Pi\varphi = \left[zA_0^{-1}(I - zA_0^{-1})^{-1} + I\right]\Pi\varphi = (I - zA_0^{-1})^{-1}\Pi\varphi = S_z\varphi.$$

The last statement is easily verified by the direct calculation based on the resolvent identity

$$\begin{aligned}
(I - zA_0^{-1})^{-1} &- (I - \zeta A_0^{-1})^{-1} \\
&= z(A_0 - zI)^{-1} - \zeta(A_0 - \zeta I)^{-1} \\
&= (A_0 - zI)^{-1}\left(zI - \zeta(I - zA_0^{-1})(I - \zeta A_0^{-1})^{-1}\right) \\
&= (A_0 - zI)^{-1}\left(z(I - \zeta A_0^{-1}) - \zeta(I - zA_0^{-1})\right)(I - \zeta A_0^{-1})^{-1} \\
&= (z - \zeta)(A_0 - zI)^{-1}(I - \zeta A_0^{-1})^{-1}.
\end{aligned}$$

Multiplication by Π from the right concludes the proof. □

Now an analogue of the “second boundary operator” γ_1 described in Sect. 1 can be introduced.

Definition 3.3. *Let Λ be a linear operator in E with the domain $\mathcal{D}(\Lambda) \subset E$. Define the linear mapping Γ_1 on the subset $\mathscr{D} := \mathcal{D}(A_0) \dot{+} \Pi\mathcal{D}(\Lambda)$ by*

$$\Gamma_1 : A_0^{-1} f + \Pi\varphi \mapsto \Pi^* f + \Lambda\varphi, \quad f \in H, \varphi \in \mathcal{D}(\Lambda). \tag{3.6}$$

Note that according to this definition $\Lambda = \Gamma_1\Pi$ and $\Pi = (\Gamma_1 A_0^{-1})^*$. In particular, for the solution operator $S_z = (I - zA_0^{-1})^{-1}\Pi = A_0(A_0 - zI)^{-1}\Pi$ we obtain

$$(S_{\bar{z}})^* = \Gamma_1(A_0 - zI)^{-1} = \Gamma_1 R_z, \quad z \in \rho(A_0). \tag{3.7}$$

Assumption 2. *Operator $\Lambda = \Gamma_1\Pi$ is selfadjoint (and thereby densely defined).*

Remark 3.4. In the sequel it is always assumed that the set $\{A_0^{-1}, \Pi, \Lambda\}$ satisfies both Assumptions 1 and 2.

Theorem 3.2 (Green's Formula).

$$(Au, v)_H - (u, Av)_H = (\Gamma_1 u, \Gamma_0 v)_E - (\Gamma_0 u, \Gamma_1 v)_E, \quad u, v \in \mathscr{D}.$$

Proof. Let $u = A_0^{-1} f + \Pi\varphi$, $v = A_0^{-1} g + \Pi\psi$ with $f, g \in H$, $\varphi, \psi \in \mathcal{D}(\Lambda)$. We have $Au = f$, $Av = g$, and due to selfadjointness of A_0^{-1} and Λ,

$$\begin{aligned}(Au, v)_H - (u, Av)_H &= (f, A_0^{-1} g + \Pi\psi) - (A_0^{-1} f + \Pi\varphi, g) \\ &= (f, \Pi\psi) - (\Pi\varphi, g) \\ &= (\Pi^* f, \psi) - (\varphi, \Pi^* g) \\ &= (\Pi^* f + \Lambda\varphi, \psi) - (\varphi, \Pi^* g + \Lambda\psi) \\ &= (\Gamma_1 u, \Gamma_0 v) - (\Gamma_0 \varphi, \Gamma_1 v)\end{aligned}$$

since both Assumptions 1 and 2 are valid. □

Introduction of the second boundary operator Γ_1 and Theorem 3.2 lead to the concept of weak solutions to the problem (3.3) defined as solutions to a certain "variational" problem.

Definition 3.4. *The weak solution of the problem* (3.3) *is an element $w_z^{f,\varphi} \in H$ satisfying*

$$(w_z^{f,\varphi}, (A_0 - \bar{z}I)v) = (f, v) + (\varphi, \Gamma_1 v) \quad \textit{for any } v \in \mathcal{D}(A_0). \tag{3.8}$$

Let us verify that this definition is consistent with the solvability statement of Theorem 3.1. In other words, we need to show that for $z \in \rho(A_0)$ the vector $u_z^{f,\varphi}$ from (3.4) solves the variational problem (3.8). Indeed, for $u_z^{f,\varphi} = R_z f + S_z\varphi$ and any $v \in \mathcal{D}(A_0)$ we have

$$\begin{aligned}(u_z^{f,\varphi}, (A_0 - \bar{z}I)v) &= (R_z f, (A_0 - \bar{z}I)v) + (S_z\varphi, (A_0 - \bar{z}I)v) \\ &= (f, v) + (\varphi, (S_z)^*(A_0 - \bar{z}I)v = (f, v) + (\varphi, \Gamma_1 v),\end{aligned}$$

according to (3.7), and the claim is proved.

Remark 3.5. The notion of weak solution suggests that the applicability of representation (3.4) is wider than that described in Theorem 3.1. Firstly, rewrite the right-hand side of 3.8 as

$$(f, v)_H + (\varphi, \Gamma_1 v)_E = (A_0^{-1} f, A_0 v) + (\varphi, \Pi^* A_0 v) = (A_0^{-1} f + \Pi\varphi, A_0 v). \qquad (3.9)$$

Recall now that $\mathcal{R}(A_0) = H$. Therefore the concept of weak solutions can be extended to the case when f and φ are chosen from spaces wider than H and E as long as the sum $A_0^{-1} f + \Pi\varphi$ belongs to H. As an illustration consider a simple example when f and φ are such that both summands on the left side of (3.9) are finite. Let $H_- \supset H$ and $E_- \supset E$ be Hilbert spaces obtained by completion of H and E with respect to norms $\|f\|_- = \|A_0^{-1} f\|_H$ and $\|\varphi\|_- = \|\Pi\varphi\|_H$, where $f \in H$, $\varphi \in E$, correspondingly. Since both $\mathrm{Ker}(A_0^{-1})$ and $\mathrm{Ker}(\Pi)$ are trivial, these norms are non-degenerate. For each $v \in \mathcal{D}(A_0)$ the usual estimates hold

$$|(f, v)| \le \|A_0^{-1} f\| \cdot \|A_0 v\| = \|f\|_- \cdot \|A_0 v\|$$

$$|(\varphi, \Gamma_1 v)| = |(\varphi, \Gamma_1 A_0^{-1} A_0 v)| = |(\Pi\varphi, A_0 v)| \le \|\Pi\varphi\| \cdot \|A_0 v\| = \|\varphi\|_- \cdot \|A_0 v\|.$$

Thus the right-hand side of (3.9) is finite for any $v \in \mathcal{D}(A_0)$ so that $A_0^{-1} f + \Pi\varphi \in H$ as long as $f \in H_-$ and $\varphi \in E_-$. It follows that the vector $u_z^{f,\varphi} = R_z f + S_z \varphi$ defined for $z \in \rho(A_0)$ by the formula (3.4) is the weak solution of (3.3) with $f \in H_-$, $\varphi \in E_-$.

Introduce the notion of M-function (M-operator) as follows.

Definition 3.5. *Operator-valued function $M(z)$ defined on the domain $\mathcal{D}(\Lambda)$ for $z \in \rho(A_0)$ by the formula*

$$M(z)\varphi = \Gamma_1 S_z \varphi = \Gamma_1 (I - z A_0^{-1})^{-1} \Pi\varphi$$

is called the M-function of the problem (3.3).

Theorem 3.3. 1. *The representation is valid*

$$M(z) = \Lambda + z\Pi^* (I - z A_0^{-1})^{-1} \Pi, \quad z \in \rho(A_0). \qquad (3.10)$$

2. *For each $\varphi \in \mathcal{D}(\Lambda)$ the vector function $M(z)\varphi$, $z \in \rho(A_0)$ with values in E is analytic for.*
3. *For $z, \zeta \in \rho(A_0)$ the operator $M(z) - M(\zeta)$ is bounded and*

$$M(z) - M(\zeta) = (z - \zeta)(S_{\bar{z}})^* S_\zeta.$$

   In particular, $\mathrm{Im}\, M(z) = (\mathrm{Im}\, z)(S_{\bar{z}})^* S_z$ *and* $(M(z))^* = M(\bar{z})$ *where* $\mathrm{Im}\, M(\cdot)$ *denotes the imaginary part of operator $M(\cdot)$.*
4. *For $u_z \in \mathrm{Ker}(A - zI) \cap \mathscr{D} = \mathrm{Ker}(A - zI) \cap \{\mathcal{D}(A_0) \dot{+} \Pi\mathcal{D}(\Lambda)\}$ the following formula holds:*

$$M(z)\Gamma_0 u_z = \Gamma_1 u_z. \qquad (3.11)$$

Proof. (1) The claim follows from the identities $\Lambda = \Gamma_1 \Pi$, $\Pi^* = \Gamma_1 A_0^{-1}$, the elementary computation

$$(I - z A_0^{-1})^{-1} = I + z(A_0 - zI)^{-1} = I + z A_0^{-1} (I - z A_0^{-1})^{-1}, \quad z \in \rho(A_0)$$

and the definition $M(z) = \Gamma_1(I - zA_0^{-1})^{-1}\Pi$.

(2) As the term $z\Pi^*(I - zA_0^{-1})^{-1}\Pi$ is a bounded analytic operator-function of $z \in \rho(A_0)$ the statement is a consequence of the representation obtained in (1).

(3) We have

$$\begin{aligned} M(z) - M(\zeta) &= \Pi^* \left[z(I - zA_0^{-1})^{-1} - \zeta(I - \zeta A_0^{-1})^{-1}\right]\Pi \\ &= \Pi^*(I - zA_0^{-1})^{-1}\left[z(I - \zeta A_0^{-1}) - \zeta(I - zA_0^{-1})\right](I - \zeta A_0^{-1})^{-1}\Pi \\ &= (z - \zeta)\Pi^*(I - zA_0^{-1})^{-1}(I - \zeta A_0^{-1})^{-1}\Pi = (z - \zeta)\left(S_{\bar{z}}\right)^* S_\zeta. \end{aligned}$$

The equality $(M(z))^* = M(\bar{z})$ is valid due to selfadjointness of Λ.

(4) Any vector $u_z \in \operatorname{Ker}(A - zI)$ is uniquely represented in the form $u_z = S_z\Gamma_0 u_z$. In the case $u_z \in \mathscr{D}$ either side belongs to $\mathcal{D}(\Gamma_1)$. Therefore, $\Gamma_1 u_z = \Gamma_1 S_z \Gamma_0 u_z = M(z)\Gamma_0 u_z$. □

Remark 3.6. Results of [22] suggest an alternative approach to build the framework described in this section. As an illustration of this possibility, and in order to explain relationships between [22] and the present paper, let us derive the representation (3.10) for Weyl function $M(z)$ within the scope of [22]. The key component here is the Example 6.6 of [22]. Using notations of this example, substitution of $D = A_0^{-1}$, $B = \Pi$, and $E = -\Lambda$ yields the following form of boundary relation $\Gamma : H \oplus H \to E \oplus E$

$$\Gamma = \left\{ \begin{pmatrix} f \\ A_0^{-1}f + \Pi\varphi \end{pmatrix}, \begin{pmatrix} \varphi \\ -\Lambda\varphi - \Pi^* f \end{pmatrix} \right\}, \quad f \in H,\ \varphi \in \mathcal{D}(\Lambda).$$

Formula *(3.6)* of [22] splits Γ into two boundary mappings, $\widehat{\Gamma_0}$ and $\widehat{\Gamma_1}$

$$\widehat{\Gamma_0} = \left\{ \begin{pmatrix} f \\ A_0^{-1}f + \Pi\varphi \end{pmatrix}, \begin{pmatrix} \varphi \\ 0 \end{pmatrix} \right\}, \quad \widehat{\Gamma_1} = \left\{ \begin{pmatrix} f \\ A_0^{-1}f + \Pi\varphi \end{pmatrix}, \begin{pmatrix} 0 \\ -\Lambda\varphi - \Pi^* f \end{pmatrix} \right\}$$

where $f \in H$, $\varphi \in \mathcal{D}(\Lambda)$. Note that the mapping $\widehat{\Gamma_0}$ can be extended to the subset $\{f, A_0^{-1}f + \Pi\varphi\}$ with $f \in H$, $\varphi \in E$. Comparison to expressions (3.2) and (3.6) for operators Γ_0 and Γ_1 clarifies relationships between $\{\widehat{\Gamma_0}, \widehat{\Gamma_1}\}$ and $\{\Gamma_0, \Gamma_1\}$. More precisely, for $f \in H$, $\varphi \in \mathcal{D}(\Lambda)$

$$\begin{aligned} \widehat{\Gamma_0} &= \left\{ \begin{pmatrix} f \\ A_0^{-1}f + \Pi\varphi \end{pmatrix}, \begin{pmatrix} \Gamma_0\left(A_0^{-1}f + \Pi\varphi\right) \\ 0 \end{pmatrix} \right\}, \\ \widehat{\Gamma_1} &= \left\{ \begin{pmatrix} f \\ A_0^{-1}f + \Pi\varphi \end{pmatrix}, \begin{pmatrix} 0 \\ -\Gamma_1\left(A_0^{-1}f + \Pi\varphi\right) \end{pmatrix} \right\}. \end{aligned}$$

Weyl family $\widehat{M}(z)$ corresponding to Γ is the relation

$$\widehat{M}(\lambda) = \left\{ \widehat{\varphi} \in E \oplus E \mid \{\widehat{f}_\lambda, \widehat{\varphi}\} \in \Gamma \text{ for some } \widehat{f}_\lambda = \{f, \lambda f\} \in H \oplus H \right\}$$

*(*see [22, Definition 3.3]*)*. For any element $\widehat{f}_\lambda = \{f, \lambda f\} \in H \oplus H$ the condition $\{\widehat{f}_\lambda, \widehat{\varphi}\} \in \Gamma$ implies $\widehat{f}_\lambda \in \mathcal{D}(\Gamma)$, which leads to the equation $\lambda f = A_0^{-1}f + \Pi\varphi$

for vectors f and φ. It follows that $f = (\lambda I - A_0^{-1})^{-1}\Pi\varphi$ at least for $\operatorname{Im}(\lambda) \neq 0$. If this equality holds, then the relation Γ takes the form

$$\Gamma = \left\{ \begin{pmatrix} f \\ \lambda f \end{pmatrix}, \begin{pmatrix} \varphi \\ -\Lambda\varphi - \Pi^*(\lambda I - A_0^{-1})^{-1}\Pi\varphi \end{pmatrix} \right\}, \quad f \in H,\, \varphi \in \mathcal{D}(\Lambda),$$

and therefore the Weyl family is the relation defined for $\varphi \in \mathcal{D}(\Lambda)$ as

$$\widehat{M}(\lambda) = \left\{ \varphi, -(\Lambda + \Pi^*(\lambda I - A_0^{-1})^{-1}\Pi)\varphi \right\}.$$

Additionally, decomposition of Γ into two boundary mappings $\widehat{\Gamma_0}$ and $\widehat{\Gamma_1}$ yields

$$\widehat{\Gamma_0} = \left\{ \begin{pmatrix} f \\ \lambda f \end{pmatrix}, \begin{pmatrix} \varphi \\ 0 \end{pmatrix} \right\}, \quad \widehat{\Gamma_1} = \left\{ \begin{pmatrix} f \\ \lambda f \end{pmatrix}, \begin{pmatrix} 0 \\ -(\Lambda + \Pi^*(\lambda I - A_0^{-1})^{-1}\Pi)\varphi \end{pmatrix} \right\},$$

and therefore $\widehat{\Gamma_1}\widehat{f_\lambda} = \widehat{M}(\lambda)\widehat{\Gamma_0}\widehat{f_\lambda}$ for any $\widehat{f_\lambda} = \{f, \lambda f\} \in \mathcal{D}(\Gamma)$ (cf. [22, Eq. (3.7)] and (3.11) above).

Finally, the relation $\widehat{M}(\lambda)$ is the graph of a linear operator in E (also denoted $\widehat{M}(\lambda)$) with the domain $\mathcal{D}(\Lambda)$ and $M(z) = -\widehat{M}(1/z)$, $\operatorname{Im}(z) \neq 0$ where $M(z)$ is the M-function (3.10) of boundary value problem (3.3).

4. Boundary Conditions

This section explores other types of boundary value problems for the operator A and boundary mappings Γ_0, Γ_1 introduced in Sect. 3. The problems under consideration are defined in terms of certain linear "boundary conditions." More precisely, given two linear operators β_0, β_1 acting in the space E we are formally looking for solutions to the equation $(A - zI)u = f$ satisfying condition $(\beta_0\Gamma_0 + \beta_1\Gamma_1)u = \varphi$ where $f \in H$, $\varphi \in E$, and $z \in \mathbb{C}$. The exact meaning of this problem statement and the solvability theorem are the main results of this section. Definitions and some properties of associated M-functions are also briefly reviewed.

Everywhere below β_0, β_1 are two linear operators in E such that β_0 is defined on the domain $\mathcal{D}(\beta_0) \supset \mathcal{D}(\Lambda)$ and β_1 is defined everywhere on E and bounded. Consider the following spectral boundary value problem for $w \in H$ associated with the set $\{A_0^{-1}, \Pi, \Lambda\}$ and the pair (β_0, β_1)

$$\begin{cases} (A - zI)w = f, \\ (\beta_0\Gamma_0 + \beta_1\Gamma_1)w = \varphi, \end{cases} \qquad f \in H, \varphi \in E, \tag{4.1}$$

where $z \in \mathbb{C}$ plays the role of a spectral parameter.

The first goal in the study of (4.1) is clarification of the equality $(\beta_0\Gamma_0 + \beta_1\Gamma_1)w = \varphi$. Having this objective in mind, observe that the sum $\beta_0\Gamma_0 + \beta_1\Gamma_1$ is defined at least on $S_z\mathcal{D}(\Lambda)$ for $z \in \rho(A_0)$ and

$$(\beta_0\Gamma_0 + \beta_1\Gamma_1)S_z\varphi = (\beta_0 + \beta_1 M(z))\,\varphi, \quad \varphi \in \mathcal{D}(\Lambda), \tag{4.2}$$

according to the properties of S_z and definition of $M(z)$. Rewrite the right-hand side using the representation $M(z) = \Lambda + z\Pi^*(I - zA_0^{-1})^{-1}\Pi$ in the form

$$(\beta_0\Gamma_0 + \beta_1\Gamma_1)S_z\varphi = (\beta_0 + \beta_1\Lambda)\varphi + z\Pi^*(I - zA_0^{-1})^{-1}\Pi\varphi, \quad \varphi \in \mathcal{D}(\Lambda). \tag{4.3}$$

The second term on the right is bounded for $z \in \rho(A_0)$, thus the mapping properties of the sum $\beta_0\Gamma_0 + \beta_1\Gamma_1$ as an operator from H into E are fully determined by the map $\beta_0 + \beta_1\Lambda$. The following closability condition is assumed to be always satisfied.

Assumption 3. *The operator $\beta_0 + \beta_1\Lambda$ defined on $\mathcal{D}(\Lambda)$ is closable in E. Let $\mathscr{B} = \overline{\beta_0 + \beta_1\Lambda}$ be its closure.*

Remark 4.1. It follows from (4.2) and (4.3) that under this assumption all operators $\beta_0 + \beta_1 M(z)$ are also closable for $z \in \rho(A_0)$ and the domain of their closures coincides with $\mathcal{D}(\mathscr{B})$. Equality (4.3) therefore can be extended to the set $\varphi \in \mathcal{D}(\mathscr{B})$. However, the operator sum $\beta_0\Gamma_0 + \beta_1\Gamma_1$ needs not be closed on the linear set $\{S_z\varphi \mid \varphi \in \mathcal{D}(\mathscr{B})\}$ and in general cannot be treated as a sum of two separate operators, $\beta_0\Gamma_0$ and $\beta_1\Gamma_1$.

Definition 4.1. *Let $\mathscr{H}_{\mathscr{B}}$ be the linear set of elements*

$$\mathscr{H}_{\mathscr{B}} = \left\{A_0^{-1}f + \Pi\varphi \mid f \in H, \varphi \in \mathcal{D}(\mathscr{B})\right\}.$$

Notice that since $\mathcal{D}(\Lambda) \subseteq \mathcal{D}(\mathscr{B}) \subseteq E$, the inclusions $\mathscr{D} \subseteq \mathscr{H}_{\mathscr{B}} \subseteq \mathcal{D}(A)$ hold, where $\mathscr{D} = \{A_0^{-1}f + \Pi\varphi \mid f \in H, \varphi \in \mathcal{D}(\Lambda)\}$, as defined in Sect. 3.

The set $\mathscr{H}_{\mathscr{B}}$ can be turned into a (closed) Hilbert space by introducing a certain non-degenerate metric. Then the map $\beta_0\Gamma_0+\beta_1\Gamma_1$ is bounded as an operator from $\mathscr{H}_{\mathscr{B}}$ into E. More precise result is given by the following Lemma.

Lemma 4.1. *The set $\mathscr{H}_{\mathscr{B}}$ is a Hilbert space with the norm*

$$\|u\|_{\mathscr{B}} = \left(\|f\|_H^2 + \|\varphi\|_E^2 + \|\mathscr{B}\varphi\|^2\right)^{1/2}.$$

The operator $\beta_0\Gamma_0 + \beta_1\Gamma_1 : \mathscr{H}_{\mathscr{B}} \to E$ is bounded.

Proof. The proof is based on the density of $\mathcal{D}(\Lambda)$ in the domain $\mathcal{D}(\mathscr{B})$ equipped with the graph norm of operator $\mathscr{B}$, which in turn implies density of $\mathscr{D}$ in $\mathscr{H}_{\mathscr{B}}$ in the norm $\|\cdot\|_{\mathscr{B}}$.

Let $\{u_n\}_{n=1}^{\infty} \subset \mathscr{D}$ be a Cauchy sequence in the norm of $\mathscr{H}_{\mathscr{B}}$, that is $\|u_n - u_m\|_{\mathscr{B}} \to 0$ as $n, m \to \infty$. Each vector u_n is represented as the sum $u_n = A_0^{-1}f_n + \Pi\varphi_n$ with uniquely defined $f_n \in H$, $\varphi_n \in \mathcal{D}(\Lambda)$. We have

$$\|u_n - u_m\|_{\mathscr{B}}^2 = \|f_n - f_m\|^2 + \|\varphi_n - \varphi_m\|^2 + \|\mathscr{B}(\varphi_n - \varphi_m)\|^2 \to 0 \ \text{ as } n, m \to \infty.$$

The first summand here tends to zero, and therefore $f_n \to f_0 \in H$ for some $f_0 \in H$ as $n \to \infty$. The sum of second and third terms is the norm of $\varphi_n - \varphi_m$ in the graph norm of $\mathscr{B}$. Because operator $\mathscr{B}$ defined on $\mathcal{D}(\Lambda)$ is closable, there exists a vector $\varphi_0 \in \mathcal{D}(\mathscr{B})$ such that $\varphi_n \to \varphi_0$ as $n \to \infty$. The limit of the sequence $\{u_n\}_{n=1}^{\infty}$ therefore is represented in the form $A_0^{-1}f_0 + \Pi\varphi_0$ where $f_0 \in H$ and $\varphi_0 \in \mathcal{D}(\mathscr{B})$. Hence $\mathscr{H}_{\mathscr{B}}$ is closed in the norm $\|\cdot\|_{\mathscr{B}}$.

The second statement follows directly from the norm estimate for elements of $\mathscr{D}$. When $f \in H$ and $\varphi \in \mathcal{D}(\Lambda)$, the sum $u = A_0^{-1}f + \Pi\varphi$ belongs to the set $\mathcal{D}(\Gamma_0) \cap \mathcal{D}(\Gamma_1)$ and

$$\begin{aligned}(\beta_0\Gamma_0 + \beta_1\Gamma_1)u &= \beta_1\Gamma_1 A_0^{-1}f + (\beta_0\Gamma_0 + \beta_1\Gamma_1)\Pi\varphi \\ &= \beta_1\Pi^* f + (\beta_0 + \beta_1\Lambda)\varphi = \beta_1\Pi^* f + \mathscr{B}\varphi.\end{aligned}$$

Because operator $\beta_1\Pi^*$ is bounded, the following estimates hold

$$\|(\beta_0\Gamma_0 + \beta_1\Gamma_1)u\| \le C\|u\|_{\mathscr{B}}, \quad u = A_0^{-1}f + \Pi\varphi,\ f \in H,\ \varphi \in \mathcal{D}(\Lambda).$$

The set $\{A_0^{-1}f + \Pi\varphi \mid f \in H, \varphi \in \mathcal{D}(\Lambda)\}$ is dense in $\mathscr{H}_{\mathscr{B}}$; hence the operator $\beta_0\Gamma_0 + \beta_1\Gamma_1$ is bounded as a mapping from $\mathscr{H}_{\mathscr{B}}$ into E. □

Remark 4.2. The symbol $\beta_0\Gamma_0 + \beta_1\Gamma_1$ will be used for the extension of operator of Lemma 4.1 to the space $\mathscr{H}_{\mathscr{B}}$, although two terms in the sum $(\beta_0\Gamma_0 + \beta_1\Gamma_1)u$ need not exist separately for an arbitrary $u \in \mathscr{H}_{\mathscr{B}}$.

Taking Lemma 4.1 into consideration, we shall look for solutions of the problem (4.1) that belong to $\mathscr{H}_{\mathscr{B}}$.

Theorem 4.1. *Suppose $z \in \rho(A_0)$ is such that the closed operator $\overline{\beta_0 + \beta_1 M(z)}$ defined on $\mathcal{D}(\mathscr{B})$ is boundedly invertible in the space E. Then the problem* (4.1) *is uniquely solvable and the solution $w_z^{f,\varphi} \in \mathscr{H}_{\mathscr{B}}$ is given by the formula*

$$w_z^{f,\varphi} = (A_0 - zI)^{-1}f + (I - zA_0^{-1})^{-1}\Pi\Psi_z^{f,\varphi} \tag{4.4}$$

where $\Psi_z^{f,\varphi}$ is a vector from $\mathcal{D}(\mathscr{B})$

$$\Psi_z^{f,\varphi} = (\overline{\beta_0 + \beta_1 M(z)})^{-1}(\varphi - \beta_1\Pi^*(I - zA_0^{-1})^{-1}f). \tag{4.5}$$

Remark 4.3. According to this theorem the problem (4.1) is reduced to the problem (3.3) with φ replaced by the vector $\Psi_z^{f,\varphi}$ defined in (4.5). This observation makes the concept of weak solutions applicable to the problem (4.1), see Definition 3.4 and Remark 3.5.

The proof of Theorem 4.1 is given at the end of this section.

In order to discuss the notion of M-operators associated with the boundary value problem (4.1) define the corresponding M-operators as follows. The solution $w_z^{\varphi} := w_z^{0,\varphi}$ is obtained in the closed form by putting $f = 0$ in (4.1) and (4.4):

$$w_z^{\varphi} = (I - zA_0^{-1})^{-1}\Pi(\overline{\beta_0 + \beta_1 M(z)})^{-1}\varphi = S_z(\overline{\beta_0 + \beta_1 M(z)})^{-1}\varphi$$

Vector w_z^{φ} belongs to the domain of Γ_0 for any $\varphi \in E$ and

$$\Gamma_0 w_z^{\varphi} = (\overline{\beta_0 + \beta_1 M(z)})^{-1}\varphi$$

Hence the operator $(\overline{\beta_0 + \beta_1 M(z)})^{-1}$ could be termed "$(\beta_0\beta_1)$-to-$(I,0)$ map." The notation "$(I,0)$" reflects equalities $\beta_0 = I$, $\beta_1 = 0$ that correspond to the condition $\Gamma_0 w = 0$ in (4.1). At the same time the inclusion $w_z^{\varphi} \in \mathcal{D}(\Gamma_1)$ needs not be valid for an arbitrary $\varphi \in E$. However, if there exists a set of $\varphi \in E$ such that vectors $(\overline{\beta_0 + \beta_1 M(z)})^{-1}\varphi$ lie in $\mathcal{D}(\Lambda)$, similar arguments lead to the definition of $(\beta_0\beta_1)$-to-$(0, I)$ map $M(z)(\overline{\beta_0 + \beta_1 M(z)})^{-1}$ that may be unbounded and even non-densely defined as an operator in E.

This argumentation is easily extendable to the definition of M-operators as $(\beta_0\beta_1)$-to-$(\alpha_0\alpha_1)$-maps, where α_0, α_1 is another pair of "boundary operators" from the boundary condition $(\alpha_0\Gamma_0 + \alpha_1\Gamma_1)u = \psi$. Such a map is formally given by the "linear-fractional transformation with operator coefficients"

$$(\alpha_0 + \alpha_1 M(z))(\overline{\beta_0 + \beta_1 M(z)})^{-1}.$$

The precise meaning of this formula needs to be clarified in each particular case at hand. Operator transformations of this kind (with z-dependent coefficients) are typical in the systems theory where M-functions are realized as transfer functions of linear systems, see [73, 77]. For the cases when $\mathrm{Ker}(\overline{\beta_0 + \beta_1 M(z)}) \neq \{0\}$ relevant results are given by the boundary triplets approach in [21, 23, 25] in terms of linear boundary relations in Hilbert and Krein spaces.

The section concludes with the proof of Theorem 4.1.

Proof. As clarified in Remark 4.1 and Remark 4.3, operators $\beta_0 + \beta_1 M(z)$ are closed on $\mathcal{D}(\mathscr{B})$ simultaneously for all $z \in \rho(A_0)$ and in accordance with Theorem 3.1 the vector $w_z^{f,\varphi}$ from (4.4), (4.5) is a solution to the system (3.3) with φ replaced by $\Psi_z^{f,\varphi}$. In particular, Theorem 3.1 implies that $\Gamma_0 w_z^{f,\varphi} = \Psi_z^{f,\varphi}$ and the solution $w_z^{f,\varphi} \in \mathrm{Ker}(A - zI)$ is unique.

Assume the vector $\Psi_z^{f,\varphi}$ defined by (4.5) belongs to $\mathcal{D}(\Lambda)$ so that $w_z^{f,\varphi} \in \mathcal{D}(\Gamma_1)$. Then

$$\Gamma_1 w_z^{f,\varphi} = \Gamma_1(A_0 - zI)^{-1}f + \Gamma_1(I - zA_0^{-1})^{-1}\Pi\Psi_z^{f,\varphi} = \Pi^*(I - zA_0^{-1})^{-1}f + M(z)\Psi_z^{f,\varphi}.$$

Therefore

$$\begin{aligned}(\beta_0\Gamma_0 + \beta_1\Gamma_1)w_z^{f,\varphi} &= (\beta_0 + \beta_1 M(z))\Psi_z^{f,\varphi} + \beta_1\Pi^*(I - zA_0^{-1})^{-1}f \\ &= \varphi - \beta_1\Pi^*(I - zA_0^{-1})^{-1}f + \beta_1\Pi^*(I - zA_0^{-1})^{-1}f = \varphi.\end{aligned}$$

Hence both equations (4.1) are satisfied if $\Psi_z^{f,\varphi} \in \mathcal{D}(\Lambda)$.

In the general case when $\Psi_z^{f,\varphi} \in \mathcal{D}(\mathscr{B})$ the vector $w_z^{f,\varphi}$ from (4.4) belongs to $\mathscr{H}_{\mathscr{B}}$ and therefore the expression $(\beta_0\Gamma_0 + \beta_1\Gamma_1)w_z^{f,\varphi}$ is well defined in accordance with Lemma 4.1. We need only show that it is equal to φ, as required by the second equation in (4.1). Consider the sequence $\Psi_n \in \mathcal{D}(\Lambda)$, $n = 0, 1, \dots$ such that $\Psi_n \to \Psi_z^{f,\varphi}$ in the graph norm of operator $\mathscr{B}$. Then vectors $w_n \in \mathscr{D}$ defined by (4.4) with $\Psi_z^{f,\varphi}$ replaced by Ψ_n converge to $w_z^{f,\varphi}$ in the metric of $\mathscr{H}_{\mathscr{B}}$ as $n \to \infty$. Due to the boundedness of expression $(\beta_0\Gamma_0 + \beta_1\Gamma_1)$ as an operator from $\mathscr{H}_{\mathscr{B}}$ to E,

$$\lim_{n\to\infty}(\beta_0\Gamma_0 + \beta_1\Gamma_1)w_n = (\beta_0\Gamma_0 + \beta_1\Gamma_1)w_z^{f,\varphi}. \tag{4.6}$$

From the other side,

$$\begin{aligned}(\beta_0\Gamma_0 + \beta_1\Gamma_1)w_n &= (\beta_0\Gamma_0 + \beta_1\Gamma_1)[(A_0 - zI)^{-1}f + (I - zA_0^{-1})^{-1}\Pi\Psi_n] \\ &= \beta_0\Psi_n + \beta_1\Gamma_1(A_0 - zI)^{-1}f + \beta_1 M(z)\Psi_n.\end{aligned}$$

Since $\beta_0\Psi_n + \beta_1 M(z)\Psi_n \to (\overline{\beta_0 + \beta_1 M(z)})\Psi_z^{f,\varphi}$ as $n \to \infty$, we see that

$$\lim_{n\to\infty}(\beta_0\Gamma_0 + \beta_1\Gamma_1)w_n = (\overline{\beta_0 + \beta_1 M(z)})\Psi_z^{f,\varphi} + \beta_1\Gamma_1(A_0 - zI)^{-1}f.$$

Direct substitution of $\Psi_z^{f,\varphi}$ from (4.5) yields $(\beta_0\Gamma_0 + \beta_1\Gamma_1)w_n \to \varphi$ as $n \to \infty$. In accordance with (4.6), the equality $(\beta_0\Gamma_0 + \beta_1\Gamma_1)w_z^{f,\varphi} = \varphi$ follows. □

5. Linear Operators of Boundary Value Problems

Let A_{00} be the minimal operator defined as a restriction of A to the set of elements $u \in \mathscr{D}$ satisfying conditions $\Gamma_0 u = \Gamma_1 u = 0$. This section is concerned with extensions of A_{00} to operators corresponding to "boundary conditions" of the form $(\beta_0\Gamma_0 + \beta_1\Gamma_1)u = 0$. These operators are first defined via their resolvents given by a version of Krein's resolvent formula [44, 48]. More conventional definitions via boundary conditions are provided in terms of extensions of A_{00}. The groundwork for the study is laid down in Theorem 4.1.

Definition 5.1. *Let A_{00} be the restriction of A_0 to the linear set*

$$\mathcal{D}(A_{00}) = \operatorname{Ker}(\Gamma_0) \cap \operatorname{Ker}(\Gamma_1) = \mathcal{D}(A_0) \cap \operatorname{Ker}(\Gamma_1),$$

that is, $A_{00} = A\big|_{\mathcal{D}(A_{00})}$. We call A_{00} the minimal operator.

The next characterization of $\mathcal{D}(A_{00})$ is more universal since it does not involve the map Γ_1. Recall that $\operatorname{Ker}(A) = \mathcal{R}(\Pi)$ by definition of A.

Remark 5.1. The domain $\mathcal{D}(A_{00})$ is described as follows

$$\mathcal{D}(A_{00}) = \{u \in \mathcal{D}(A_0) \mid A_0 u \perp \mathcal{R}(\Pi)\} = A_0^{-1}\left(\mathcal{R}(\Pi)^{\perp}\right)$$

where $\mathcal{R}(\Pi)^{\perp}$ is the orthogonal complement to the range of Π. The range of A_{00} is closed in H and coincides with the subspace $\mathcal{R}(\Pi)^{\perp} = H \ominus \overline{\operatorname{Ker}(A)}$.

Proof. Indeed, if $u \in \mathcal{D}(A_0)$ then $u = A_0^{-1}f$ with some $f \in H$. The condition $\Gamma_1 u = 0$ means that $\Gamma_1 A_0^{-1} f = 0$, or $f \in \operatorname{Ker}(\Pi^*)$ (since $\Gamma_1 A_0^{-1} = \Pi^*$), which is equivalent to $f \perp \mathcal{R}(\Pi)$. The second statement holds because $A_{00}A_0^{-1}\mathcal{R}(\Pi)^{\perp} = \mathcal{R}(\Pi)^{\perp} = H \ominus \overline{\operatorname{Ker} A}$. □

Remark 5.2. The equality $\mathcal{D}(A_{00}) = A_0^{-1}\mathcal{R}(\Pi)^{\perp}$ shows in particular that the operator A_{00} does not depend on any given choice of Λ. Moreover, A_{00} is symmetric but need not be densely defined. The operator A_0 is a selfadjoint extension of A_{00} contained in A.

Relations (4.5) and (4.4) offer a rather natural way to define the resolvent of an operator associated with the "boundary condition" $(\beta_0\Gamma_0 + \beta_1\Gamma_1)u = 0$. By putting $\varphi = 0$ and inserting (4.5) into (4.4) a suitable candidate for the role of resolvent is obtained:

$$\begin{aligned}&\mathscr{R}_{\beta_0,\beta_1}(z)\\ &\quad = (A_0 - zI)^{-1} - (I - zA_0^{-1})^{-1}\Pi(\overline{\beta_0 + \beta_1 M(z)})^{-1}\beta_1\Pi^*(I - zA_0^{-1})^{-1}.\end{aligned} \tag{5.1}$$

As will be shown, the operator function (5.1) is indeed the resolvent of some closed linear operator A_{β_0,β_1} in H whose domain $\mathcal{D}(A_{\beta_0,\beta_1})$ coincides with the set $\operatorname{Ker}(\beta_0\Gamma_0+\beta_1\Gamma_1)$. Assuming the conditions of Theorem 4.1 are satisfied, denote

$$Q_{\beta_0,\beta_1}(z) = -(\overline{\beta_0+\beta_1 M(z)})^{-1}\beta_1.$$

The operator-function $Q_{\beta_0,\beta_1}(z)$ is analytic and bounded as long as $z\in\rho(A_0)$ satisfies conditions of Theorem 4.1. The expression (5.1) for $\mathscr{R}_{\beta_0,\beta_1}(z)$ takes the form

$$\mathscr{R}_{\beta_0,\beta_1}(z) = R_z + S_z Q_{\beta_0,\beta_1}(z) S^*_{\bar z} \tag{5.2}$$

where $R_z=(A_0-zI)^{-1}$ is the resolvent of A_0 and $S_z=(I-zA_0^{-1})^{-1}\Pi$ is the solution operator. For simplicity, the indices in Q_{β_0,β_1} will be omitted and the notation $Q(z)$ will be used for $Q_{\beta_0,\beta_1}(z)$ when it does not lead to confusion. An important analytical property of $Q(z)$ is formulated in the next lemma.

Lemma 5.1. *For $z,\zeta\in\rho(A_0)$ satisfying assumptions of Theorem 4.1 the following equality holds:*

$$Q(z)-Q(\zeta) = (z-\zeta)Q(z)S^*_{\bar z}S_\zeta Q(\zeta).$$

Proof. By virtue of formula (3) from Theorem 3.3, we have for $\varphi\in\mathcal{D}(\Lambda)$

$$\begin{aligned}
&(z-\zeta)\beta_1 S^*_{\bar z}S_\zeta\varphi\\
&\quad=\beta_1\left[M(z)-M(\zeta)\right]\varphi\\
&\quad=(\overline{\beta_0+\beta_1M(z)})\varphi-(\overline{\beta_0+\beta_1M(\zeta)})\varphi\\
&\quad=(\overline{\beta_0+\beta_1M(z)})\left[(\overline{\beta_0+\beta_1M(\zeta)})^{-1}-(\overline{\beta_0+\beta_1M(z)})^{-1}\right](\overline{\beta_0+\beta_1M(\zeta)})\varphi.
\end{aligned}$$

Therefore

$$\begin{aligned}
(z-\zeta)Q(z)S^*_{\bar z}S_\zeta Q(\zeta) &= \left[(\overline{\beta_0+\beta_1M(\zeta)})^{-1}-(\overline{\beta_0+\beta_1M(z)})^{-1}\right]\beta_1\\
&=Q(z)-Q(\zeta),
\end{aligned}$$

as stated. □

The main theorem of this section reads as follows.

Theorem 5.1. *Assume $z\in\rho(A_0)$ is such that the closed operator $\overline{\beta_0+\beta_1M(z)}$ defined on $\mathcal{D}(\mathscr{B})$ is boundedly invertible in the space E. Then the operator function $\mathscr{R}_{\beta_0,\beta_1}(z)$ defined by (5.1) is the resolvent of a closed densely defined operator A_{β_0,β_1} in H. For A_{β_0,β_1} the inclusions are valid*

$$A_{00}\subset A_{\beta_0,\beta_1}\subset A, \tag{5.3}$$

The domain of A_{β_0,β_1} satisfies

$$\mathcal{D}(A_{\beta_0,\beta_1}) = \{u\in\mathscr{H}_{\mathscr{B}} \mid (\beta_0\Gamma_0+\beta_1\Gamma_1)u=0\} = \operatorname{Ker}(\beta_0\Gamma_0+\beta_1\Gamma_1). \tag{5.4}$$

In addition,

$$\Gamma_0(A_{\beta_0,\beta_1}-zI)^{-1} = Q(z)\Gamma_1(A_0-zI)^{-1} \tag{5.5}$$

and the resolvent identity holds:

$$(A_{\beta_0,\beta_1}-zI)^{-1}-(A_0-zI)^{-1} = \left[\Gamma_1(A_0-\bar zI)^{-1}\right]^*\Gamma_0(A_{\beta_0,\beta_1}-zI)^{-1}. \tag{5.6}$$

Proof. Operator function $\mathscr{R}(z) = \mathscr{R}_{\beta_0,\beta_1}(z)$ is bounded and analytic for suitable $z \in \mathbb{C}$. To show that $\mathscr{R}(z)$ is a resolvent, we need to check three conditions [40]. They are: (1) $\mathrm{Ker}(\mathscr{R}(z)) = \{0\}$, (2) $\mathcal{R}(\mathscr{R}(z))$ is dense in H, and (3) the function $\mathscr{R}(z)$ satisfies the first resolvent equation

$$\mathscr{R}(z) - \mathscr{R}(\zeta) = (z-\zeta)\mathscr{R}(z)\mathscr{R}(\zeta). \tag{5.7}$$

The equality $\mathrm{Ker}(\mathscr{R}(z)) = \{0\}$ follows directly from the last statement of Theorem 3.1. The same argument applied to $[\mathscr{R}(z)]^*$ in conjunction with boundedness of $Q(z)$ and equality $\mathrm{Ker}([\mathscr{R}(z)]^*) = H \ominus \mathcal{R}(\mathscr{R}(z))$ shows that the range of $\mathscr{R}(z)$ is dense in H.

We shall verify the resolvent identity for $\mathscr{R}(\cdot)$ written in simplified notation (5.2):

$$\begin{aligned}\mathscr{R}(z)\mathscr{R}(\zeta) &= \left(R_z + S_z Q(z) S_{\bar z}^*\right) \times \left(R_\zeta + S_\zeta Q(\zeta) S_{\bar\zeta}^*\right)\\ &= R_z R_\zeta + R_z S_\zeta Q(\zeta) S_{\bar\zeta}^* + S_z Q(z) S_{\bar z}^* R_\zeta + S_z Q(z) S_{\bar z}^* S_\zeta Q(\zeta) S_{\bar\zeta}^*.\end{aligned}$$

Multiplying by $(z-\zeta)$ and noticing that $R_z - R_\zeta = (z-\zeta)R_z R_\zeta$ due to the resolvent identity for A_0, the identity (5.7) is rewritten as

$$\begin{aligned}S_z Q(z) S_{\bar z}^* - S_\zeta Q(\zeta) S_{\bar\zeta}^* = (z-\zeta)\Big[R_z S_\zeta Q(\zeta) S_{\bar\zeta}^* + S_z Q(z) S_{\bar z}^* R_\zeta\Big]&\\ + (z-\zeta) S_z Q(z) S_{\bar z}^* S_\zeta Q(\zeta) S_{\bar\zeta}^*.&\end{aligned}$$

By virtue of (3.5), its adjoint, and Lemma 5.1 the right-hand side of this equality is

$$(S_z - S_\zeta) Q(\zeta) S_{\bar\zeta}^* + S_z Q(z)(S_{\bar z}^* - S_{\bar\zeta}^*) + S_z(Q(z) - Q(\zeta)) S_{\bar\zeta}^*,$$

which coincides with the left-hand side. The existence of a closed densely defined operator A_{β_0,β_1} with the resolvent $(A_{\beta_0,\beta_1} - zI)^{-1}$ defined by (5.1) thereby is proven.

Turning to the proof of (5.3), notice that in accordance with (5.2) the range of $(A_{\beta_0,\beta_1} - zI)^{-1}$ is contained in $\mathcal{D}(A)$ and since $S_z f \in \mathrm{Ker}(A - zI)$ for $f \in H$,

$$(A - zI)(A_{\beta_0,\beta_1} - zI)^{-1} f = (A - zI)\left(R_z + S_z Q(z) S_{\bar z}^*\right) f = (A - zI) R_z f = f.$$

Hence $Ag = A_{\beta_0,\beta_1} g$ for $g \in \mathcal{D}(A_{\beta_0,\beta_1})$, which means $A_{\beta_0,\beta_1} \subset A$.

To prove the inclusion $\mathcal{D}(A_{\beta_0,\beta_1}) \subset \mathrm{Ker}(\beta_0\Gamma_0 + \beta_1\Gamma_1)$ in (5.4) note that, as follows from (4.5) with $\varphi = 0$, the vector $w_z^f = (A_{\beta_0,\beta_1} - zI)^{-1} f$ is represented as $(A_{\beta_0,\beta_1} - zI)^{-1} f = R_z f + S_z \Psi_z^f$ for each element $f \in H$, where $\Psi_z^f = Q(z) S_{\bar z}^* f \in \mathcal{D}(\mathscr{B})$. Therefore $w_z^f \in \mathscr{H}_{\mathscr{B}}$ and $(\beta_0\Gamma_0 + \beta_1\Gamma_1) w_z^f = 0$ by Theorem 4.1 with $\varphi = 0$. Hence $\mathcal{D}(A_{\beta_0,\beta_1})$ in included into $\mathrm{Ker}(\beta_0\Gamma_0 + \beta_1\Gamma_1)$.

In order to prove the inverse inclusion first consider $u \in \mathscr{D}$ in the form $u = R_z f + S_z \varphi \in \mathrm{Ker}(\beta_0\Gamma_0 + \beta_1\Gamma_1)$ with $f \in H$ and $\varphi \in \mathcal{D}(\Lambda)$. Then $u \in \mathcal{D}(\Gamma_0) \cap \mathcal{D}(\Gamma_1)$ and the operator sum $\beta_0\Gamma_0 + \beta_1\Gamma_1$ can be calculated for the element u termwise,

i. e. $(\beta_0\Gamma_0 + \beta_1\Gamma_1)u = \beta_0\Gamma_0 u + \beta_1\Gamma_1 u$,

$$\begin{aligned}(\beta_0\Gamma_0 + \beta_1\Gamma_1)u &= (\beta_0\Gamma_0 + \beta_1\Gamma_1)(R_z f + S_z\varphi)\\ &= \beta_0\Gamma_0 S_z\varphi + \beta_1\Gamma_1(A_0 - zI)^{-1}f + \beta_1\Gamma_1 S_z\varphi \\ &= \beta_1\Pi^*(I - zA_0^{-1})^{-1}f + (\beta_0 + \beta_1 M(z))\varphi.\end{aligned} \tag{5.8}$$

If $u \in \operatorname{Ker}(\beta_0\Gamma_0 + \beta_1\Gamma_1)$, the left hand side of (5.8) equals zero, so that

$$\varphi = -(\overline{\beta_0 + \beta_1 M(z)})^{-1}\beta_1\Pi^*(I - zA_0^{-1})^{-1}f = Q_{\beta_0,\beta_1}(z)S_{\bar z}^* f,$$

by virtue of invertibility of $\beta_0 + \beta_1 M(z)$. Thus, vector $u = R_z f + S_z\varphi$ due to (5.2) is

$$u = (R_z + S_z Q_{\beta_0,\beta_1}(z)S_{\bar z}^*)f = \mathscr{R}_{\beta_0,\beta_1}(z)f.$$

Since $\mathscr{R}_{\beta_0,\beta_1}(z)$ is the resolvent ofA_{β_0,β_1}, we have $u \in \mathcal{D}(A_{\beta_0,\beta_1})$.

Consider now the general case of element $v = R_z f + S_z\varphi \in \mathscr{H}_{\mathscr{B}}$, $f \in H$, $\varphi \in \mathcal{D}(\mathscr{B})$ so that $v \notin \mathscr{D}$ and the operator sum $\beta_0\Gamma_0 + \beta_1\Gamma_1$ calculated on v cannot be computed termwise. Since the set $\mathscr{D}$ is dense in the Hilbert space $\mathscr{H}_{\mathscr{B}}$, see Definition 4.1 and Lemma 4.1, there exists a sequence $v_n = R_z f_n + S_z\varphi_n$ with $f_n \in H$ and $\varphi_n \in \mathcal{D}(\Lambda)$ converging to v in $\mathscr{H}_{\mathscr{B}}$ as $n \to \infty$. It means in particular that $\varphi_n \to \varphi$ and $(\overline{\beta_0 + \beta_1 M(z)})\varphi_n \to (\overline{\beta_0 + \beta_1 M(z)})\varphi$ for $n \to \infty$. Because $\beta_0\Gamma_0 + \beta_1\Gamma_1$ is bounded as an operator from $\mathscr{H}_{\mathscr{B}}$ to E by virtue of Lemma 4.1, we have

$$(\beta_0\Gamma_0 + \beta_1\Gamma_1)v_n \to (\beta_0\Gamma_0 + \beta_1\Gamma_1)v, \quad n \to \infty. \tag{5.9}$$

Expression for $(\beta_0\Gamma_0 + \beta_1\Gamma_1)v_n$ follows from (5.8)

$$(\beta_0\Gamma_0 + \beta_1\Gamma_1)v_n = \beta_1\Pi^*(I - zA_0^{-1})^{-1}f_n + (\beta_0 + \beta_1 M(z))\varphi_n.$$

Because of the boundedness of $\beta_1\Pi^*(I - zA_0^{-1})^{-1}$ and closability of $\beta_0 + \beta_1 M(z)$ this leads to

$$(\beta_0\Gamma_0 + \beta_1\Gamma_1)v_n \to \beta_1\Pi^*(I - zA_0^{-1})^{-1}f + (\overline{\beta_0 + \beta_1 M(z)})\varphi, \quad n \to \infty.$$

Comparison with (5.9) gives

$$(\beta_0\Gamma_0 + \beta_1\Gamma_1)v = \beta_1\Pi^*(I - zA_0^{-1})^{-1}f + (\overline{\beta_0 + \beta_1 M(z)})\varphi.$$

Therefore if $v \in \operatorname{Ker}(\beta_0\Gamma_0 + \beta_1\Gamma_1)$, then under conditions of Theorem

$$\varphi = -(\overline{\beta_0 + \beta_1 M(z)})^{-1}\beta_1\Pi^*(I - zA_0^{-1})^{-1}f = Q_{\beta_0,\beta_1}(z)S_{\bar z}^* f.$$

Hence, $v = (R_z f + S_z Q_{\beta_0,\beta_1}(z)S_{\bar z}^*)f = \mathscr{R}_{\beta_0,\beta_1}(z)f$ and $v \in \mathcal{D}(A_{\beta_0,\beta_1})$.

To prove that $A_{00} \subset A_{\beta_0,\beta_1}$ in (5.3) we need to show that any vector u from $\mathcal{D}(A_{00})$ belongs to $\mathcal{D}(A_{\beta_0,\beta_1})$, in other words, can be represented in the form $u = (A_{\beta_0,\beta_1} - zI)^{-1}f$ with some $f \in H$. Suppose $u \in \mathcal{D}(A_{00})$ and let us choose $f = (A_{00} - zI)u$. Then $f = (A_0 - zI)u$ because $A_{00} \subset A_0$ and

$$\begin{aligned}(A_{\beta_0,\beta_1} - zI)^{-1} f &= (A_{\beta_0,\beta_1} - zI)^{-1}(A_0 - zI)u \\ &= \left(R_z + S_z Q(z) S_{\bar z}^*\right)(A_0 - zI)u \\ &= u + S_z Q(z) S_{\bar z}^*(A_0 - zI)u \\ &= u.\end{aligned}$$

The last equality holds due to identities

$$S_{\bar z}^*(A_0 - zI)u = \Pi^*(I - zA_0^{-1})^{-1}(A_0 - zI)u = \Gamma_1 u, \quad u \in \mathscr{D}.$$

and $\Gamma_1 u = 0$ for $u \in \mathcal{D}(A_{00})$. All claims (5.3) and (5.4) are proven.

Finally, in the notation above the formula (5.5) is equivalent to the already established relation $\Gamma_0 w_z^f = \Psi_z^f$. The resolvent identity (5.6) is obtained from (5.1) by (5.5) and equality $\Gamma_1(A_0 - zI)^{-1} = \Pi^*(I - zA_0^{-1})^{-1}$. □

Remark 5.3. Equalities (5.1) and (5.6) are correspondingly Krein's formula and Hilbert resolvent identity for A_0 and A_{β_0,β_1}.

Remark 5.4. Let $\widetilde{\beta}_0$ and $\widetilde{\beta}_1$ be two linear operators with the same properties as β_0 and β_1 in Theorem 5.1. A natural question arises as to whether the boundary conditions $(\widetilde{\beta}_0\Gamma_0 + \widetilde{\beta}_1\Gamma_1)u = 0$ define the same operator as the conditions $(\beta_0\Gamma_0 + \beta_1\Gamma_1)u = 0$ discussed in the theorem. One obvious answer is that when $\beta_0 = C\widetilde{\beta}_0$ and $\beta_1 = C\widetilde{\beta}_1$ with some operator C such that $\mathrm{Ker}(C) = \{0\}$ then the equality $A_{\beta_0,\beta_1} = A_{\widetilde{\beta}_0,\widetilde{\beta}_1}$ holds because the null sets $\mathrm{Ker}(\beta_0\Gamma_0 + \beta_1\Gamma_1)$ and $\mathrm{Ker}(\widetilde{\beta}_0\Gamma_0 + \widetilde{\beta}_1\Gamma_1)$ are equal. Necessary and sufficient condition follows from the formula (5.1). Namely, the identity $\Pi Q_{\beta_0,\beta_1}(z)\Pi^* = \Pi Q_{\widetilde{\beta}_0,\widetilde{\beta}_1}(z)\Pi^*$ for z in a *(*non-empty*)* domain of the complex plane is equivalent to the identity of resolvents of A_{β_0,β_1} and $A_{\widetilde{\beta}_0,\widetilde{\beta}_1}$, thus to the equality $A_{\beta_0,\beta_1} = A_{\widetilde{\beta}_0,\widetilde{\beta}_1}$.

Corollary 5.1. *Assume the operator* $\mathscr{B} = \overline{\beta_0 + \beta_1\Lambda}$ *is boundedly invertible in* E. *Then* A_{β_0,β_1} *is boundedly invertible in* H,

$$A_{\beta_0,\beta_1}^{-1} = A_0^{-1} - \Pi(\overline{\beta_0 + \beta_1\Lambda})^{-1}\beta_1\Pi^* = A_0^{-1} + \Pi Q(0)\Pi^*,$$

and $Q(z)$ *has the representation*

$$Q(z) = Q(0) + zQ(0)\Pi^*(I - zA_{\beta_0,\beta_1}^{-1})^{-1}\Pi Q(0)$$

at least in a small neighborhood of $z = 0$.

Proof. Noting that $Q(0) = -(\overline{\beta_0 + \beta_1\Lambda})^{-1}\beta_1$ is bounded, invertibility of A_{β_0,β_1} and the formula for A_{β_0,β_1}^{-1} follow directly from (5.1) or (5.2). Existence of $Q(z) = -(\overline{\beta_0 + \beta_1 M(z)})^{-1}\beta_1$ for small $|z|$ results from analyticity and invertibility of $\overline{\beta_0 + \beta_1 M(z)}$ at $z = 0$. Lemma 5.1 with $\zeta = 0$ yields

$$Q(z) = Q(0) + zQ(z)S_{\bar z}^* S_0 Q(0). \tag{5.10}$$

Observe now that $Q(z)S_{\bar z}^* = Q(z)\Gamma_1(A_0 - zI)^{-1}$, thus according to (5.5),

$$Q(z)S_{\bar z}^* = \Gamma_0(A_{\beta_0,\beta_1} - zI)^{-1} = \Gamma_0 A_{\beta_0,\beta_1}^{-1}(I - zA_{\beta_0,\beta_1}^{-1})^{-1}$$

Formula (5.5) for $z = 0$ gives $\Gamma_0 A^{-1}_{\beta_0,\beta_1} = Q(0)\Gamma_1 A_0^{-1} = Q(0)\Pi^*$ so that

$$Q(z)S^*_{\bar{z}} = Q(0)\Pi^*(I - zA^{-1}_{\beta_0,\beta_1})^{-1}.$$

In combination with $S_0 Q(0) = \Pi Q(0)$ the expression (5.10) yields the required representation for $Q(z)$. □

Corollary 5.2. *Assume conditions of Corollary* 5.1 *are satisfied, operators* β_0, β_1 *and* Λ *are bounded, and* $\beta_0\beta_1^*$ *is selfadjoint. Then* A_{β_0,β_1} *is selfadjoint.*

Proof. Since $A^{-1}_{\beta_0,\beta_1} - (A^{-1}_{\beta_0,\beta_1})^* = \Pi\left[(\beta_0 + \beta_1\Lambda)^{-1}\beta_1 - \beta_1^*(\beta_0^* + \Lambda\beta_1^*)^{-1}\right]\Pi^*$

$$= \Pi(\beta_0 + \beta_1\Lambda)^{-1}\left[\beta_1(\beta_0^* + \Lambda\beta_1^*) - (\beta_0 + \beta_1\Lambda)\beta_1^*\right](\beta_0^* + \Lambda\beta_1^*)^{-1}\Pi^* = 0$$

under assumption $\beta_1\beta_0^* = \beta_0\beta_1^*$, the operator A_{β_0,β_1} is an (unbounded) inverse of the bounded selfadjoint operator. □

A special case of operator A_{β_0,β_1} in Theorem 5.1 with $\beta_0 = 0$, $\beta_1 = I$ is of particular interest. It can be seen as an abstract analogue of the Laplacian with Neumann boundary condition from Sect. 2. Note that in this case $Q(z) = -(M(z))^{-1}$ and $Q(0) = -\Lambda^{-1}$.

Corollary 5.3. *Suppose* Λ *is boundedly invertible. Then operator* A_1 *defined as a restriction of* A *to the set* $\mathcal{D}(A_1) = \{u \in \mathscr{D} \mid \Gamma_1 u = 0\}$ *is selfadjoint and boundedly invertible. For* $z \in \rho(A_0) \cap \rho(A_1)$,

$$(A_1 - zI)^{-1} = (A_0 - zI)^{-1} - (I - zA_0^{-1})^{-1}\Pi(M(z))^{-1}\Pi^*(I - zA_0^{-1})^{-1} \quad (5.11)$$

where $(M(z))^{-1} = \Lambda^{-1} - z\Lambda^{-1}\Pi^*(I - zA_1^{-1})^{-1}\Pi\Lambda^{-1}$, $z \in \rho(A_1)$.

Moreover, for $z \in \rho(A_0) \cap \rho(A_1)$,

$$(A_1 - zI)^{-1} = (A_0 - zI)^{-1} - (I - zA_1^{-1})^{-1}\pi M(z)\pi^*(I - zA_1^{-1})^{-1}, \quad (5.12)$$

where $\pi = (\Gamma_0 A_1^{-1})^*$ *is bounded with* $\mathcal{R}(\pi^*) \subset \mathcal{D}(\Lambda)$.

In particular, $A_1^{-1} = A_0^{-1} - \Pi\Lambda^{-1}\Pi^* = A_0^{-1} - \pi\Lambda\pi^*$ *where both* $\Pi\Lambda^{-1}\Pi^*$ *and* $\pi\Lambda\pi^*$ *are bounded operators.*

Proof. The first equality (5.11) follows directly from (5.1) and Theorem 5.1. Selfadjointness of A_1 is a consequence of representation of A_1^{-1} as a sum of two bounded selfadjoint operators. Because A_1^{-1} is bounded, the analytic operator function $(M(z))^{-1}$ from (5.11) can be analytically continued from a neighborhood of the origin $z = 0$ to all $z \in \rho(A_1)$. The alternative representation (5.12) is obtained from (5.11) with the help of equalities (5.5) and (5.6). Boundedness of the operator function $\pi M(z)\pi^*$, $z \in \rho(A_0)$, or equivalently of the operator $\pi\Lambda\pi^*$, is ensured by the calculations

$$\pi^* = \Gamma_0 A_1^{-1} = \Gamma_0(A_0^{-1} - \Pi\Lambda^{-1}\Pi^*) = -\Gamma_0\Pi\Lambda^{-1}\Pi^* = -\Lambda^{-1}\Pi^*,$$

so that $\Lambda\pi^* = -\Pi^*$. This equality also follows from (5.5) with $z = 0$. □

There exists a close relationship between analytical properties of the operator-function $Q_{\beta_0,\beta_1}(z)$ and spectral characteristics of A_{β_0,β_1}. For example, papers [24, 25] report some general results obtained within the boundary triplet based framework when $\beta_1 = I$, β_0 is closed, $\mathcal{R}(\Gamma_0) = \mathcal{R}(\Gamma_1) = E$, and therefore $M(z)$ is bounded. The next theorem regarding the point spectrum of A_{β_0,β_1} renders similar results in the paper's setting. Much more complicated relationships between spectral properties of nonselfadjoint operators and their M-functions are discussed in [15, 17].

Theorem 5.2. *Assume the operator $\mathscr{B} = \overline{\beta_0 + \beta_1\Lambda}$ is boundedly invertible. Then for any $z \in \rho(A_0)$ the mapping $\varphi \mapsto S_z\varphi$ establishes a one-to-one correspondence between $\{\varphi \in \mathcal{D}(\mathscr{B}) \mid (\overline{\beta_0 + \beta_1 M(z)})\varphi = 0\}$ and* $\mathrm{Ker}(A_{\beta_0,\beta_1} - zI)$*. In particular,* $\mathrm{Ker}(\overline{\beta_0 + \beta_1 M(z)}) = \{0\}$ *is equivalent to* $\mathrm{Ker}(A_{\beta_0,\beta_1} - zI) = \{0\}$ *for $z \in \rho(A_0)$.*

Proof. We start with the observation that under the theorem's assumptions the operator $Q(0) = -\mathscr{B}^{-1}\beta_1$ is bounded. Hence, according to Corollary 5.1, A_{β_0,β_1} is boundedly invertible and $A^{-1}_{\beta_0,\beta_1} = A_0^{-1} + \Pi Q(0)\Pi^*$.

Assume that $(\overline{\beta_0 + \beta_1 M(z)})\varphi = 0$ for some $z \in \rho(A_0)$ and $\varphi \in \mathcal{D}(\mathscr{B})$. Let $u = S_z\varphi$ be the corresponding solution to the equation $(A - zI)u = 0$ satisfying condition $\Gamma_0 u = \varphi$. Then

$$0 = (\overline{\beta_0 + \beta_1 M(z)})\varphi = (\overline{\beta_0 + \beta_1\Lambda})\varphi + z\beta_1\Pi^*(I - zA_0^{-1})^{-1}\Pi\varphi,$$

and therefore φ can be expressed in terms of $u = (I - zA_0^{-1})^{-1}\Pi\varphi$ as follows

$$\varphi = -z(\overline{\beta_0 + \beta_1\Lambda})^{-1}\beta_1\Pi^*(I - zA_0^{-1})^{-1}\Pi\varphi = -z\mathscr{B}^{-1}\beta_1\Pi^* S_z\varphi = zQ(0)\Pi^* u$$

Owing to identity $(I - zA_0^{-1})^{-1} = I + zA_0^{-1}(I - zA_0^{-1})^{-1}$ we obtain

$$\begin{aligned} u &= (I - zA_0^{-1})^{-1}\Pi\varphi \\ &= \Pi\varphi + zA_0^{-1}(I - zA_0^{-1})^{-1}\Pi\varphi \\ &= \Pi\varphi + zA_0^{-1}S_z\varphi \\ &= z\Pi Q(0)\Pi^* u + zA_0^{-1}u = z(A_0^{-1} + \Pi Q(0)\Pi^*)u \\ &= zA^{-1}_{\beta_0,\beta_1}u. \end{aligned}$$

It means inclusion $u \in \mathcal{D}(A_{\beta_0,\beta_1})$. It follows that $(A_{\beta_0,\beta_1} - zI)u = (A - zI)u = 0$ since $A_{\beta_0,\beta_1} \subset A$.

Suppose now that $u \in \mathrm{Ker}(A_{\beta_0,\beta_1} - zI)$ and denote $\varphi = \Gamma_0 u \in E$. Then u has the form $u = (I - zA_0^{-1})^{-1}\Pi\varphi$ because $A_{\beta_0,\beta_1} \subset A$ and therefore $u \in \mathrm{Ker}(A - zI)$. We need to show that φ belongs to the domain of $\mathscr{B} = \overline{\beta_0 + \beta_1\Lambda}$ and $\mathscr{B}\varphi = -z\beta_1\Pi^* u$. The equality $(A_{\beta_0,\beta_1} - zI)u = 0$ implies $(I - zA^{-1}_{\beta_0,\beta_1})u = 0$. Hence $u = zA^{-1}_{\beta_0,\beta_1}u = z\left(A_0^{-1} + \Pi Q(0)\Pi^*\right)u$. Application of Γ_0 to both sides yields $\varphi = \Gamma_0 u = zQ(0)\Pi^* u$. Recall now that $Q(0) = -(\overline{\beta_0 + \beta_1\Lambda})^{-1}\beta_1 = -\mathscr{B}^{-1}\beta_1$ and the required identity $\mathscr{B}\varphi = -z\beta_1\Pi^* u$ follows. $\square$

The rest of this section is devoted to the special case of operators A_{β_0,β_1} inspired by the Birman–Krein–Vishik theory of extensions of positive symmetric operators [11, 44, 85]. Only a simplified version of this theory is considered assuming that the extension parameter (operator B below) is densely defined and boundedly invertible in the space $\overline{\mathcal{R}(\Pi)}$. For the general case of the Birman–Krein–Vishik theory the reader is referred, apart from the original publications cited above, to the work [35] for the exhaustive treatment and to the paper [6] for an overview.

Denote $\mathcal{H} := \overline{\mathcal{R}(\Pi)} = \overline{\mathrm{Ker}(A)}$. Recall that according to Remark 5.1 the orthogonal complement of $\mathcal{H}$ is the subspace $\mathcal{H}^\perp = H \ominus \overline{\mathrm{Ker}(A)} = \mathcal{R}(A_{00})$. Let B be a closed densely defined operator in $\mathcal{H}$ such that $\mathcal{D}(B) \supset \Pi\mathcal{D}(\Lambda)$. Consider the restriction L_B of A to the set

$$\mathcal{D}(L_B) = \left\{A_0^{-1}(f_\perp + Bh) + h \mid f_\perp \in \mathcal{H}^\perp, h \in \Pi\mathcal{D}(\Lambda)\right\}.$$

Since $L_B \subset A$ by definition, we have

$$L_B : A_0^{-1}(f_\perp + Bh) + h \mapsto f_\perp + Bh, \quad f_\perp \in \mathcal{H}^\perp,\ h \in \Pi\mathcal{D}(\Lambda). \tag{5.13}$$

Clearly, $A_{00} \subset L_B$ because $\mathcal{D}(A_{00}) = A_0^{-1}\mathcal{H}^\perp \subset \mathcal{D}(L_B)$. We would like to show that L_B is closed and $L_B = A_{\beta_0,\beta_1}$ for some β_0, β_1. To simplify the matter, additional conditions of the boundedness and invertibility of $\Pi^* B\Pi$ are imposed in the following theorem.

Theorem 5.3. *Suppose the set $B\Pi\mathcal{D}(\Lambda)$ is dense in $\mathcal{H}$ and the operator $\Pi^* B\Pi$ is bounded and boundedly invertible in E. Then the inverse L_B^{-1} exists and*

$$L_B^{-1} = A_0^{-1} + \Pi(\Pi^* B\Pi)^{-1}\Pi^*. \tag{5.14}$$

Moreover, $L_B = A_{\beta_0,\beta_1}$ with $\beta_1 = -I_E$ and $\beta_0 = \Lambda + \Pi^* B\Pi$. In particular, if the function

$$M_B(z) = \Lambda_B + z\Pi^*(I - zA_0^{-1})^{-1}\Pi, \quad \text{with} \;\; \Lambda_B = -\Pi^* B\Pi,$$

is boundedly invertible for some $z \in \rho(A_0)$, then $z \in \rho(L_B)$ and

$$(L_B - zI)^{-1} = (A_0 - zI)^{-1} - (I - zA_0^{-1})^{-1}\Pi M_B^{-1}(z)\Pi^*(I - zA_0^{-1})^{-1}.$$

Proof. Formula (5.14) is verified by direct computations.
Assuming $u = A_0^{-1}(f_\perp + B\Pi\varphi) + \Pi\varphi$ with $f_\perp \in \mathcal{H}^\perp = \mathrm{Ker}(\Pi^*)$ and $\varphi \in \mathcal{D}(\Lambda)$, we have

$$\begin{aligned}\left(A_0^{-1} + \Pi(\Pi^* B\Pi)^{-1}\Pi^*\right) L_B u &= \left(A_0^{-1} + \Pi(\Pi^* B\Pi)^{-1}\Pi^*\right)(f_\perp + B\Pi\varphi)\\ &= A_0^{-1}(f_\perp + B\Pi\varphi) + \Pi(\Pi^* B\Pi)^{-1}\Pi^* B\Pi\varphi\\ &= A_0^{-1}(f_\perp + B\Pi\varphi) + \Pi\varphi\\ &= u\end{aligned}$$

From the other side, consider $f \in H$ in the form $f = f_\perp + B\Pi\varphi$ with $f_\perp \in \mathscr{H}^\perp$, $\varphi \in \mathcal{D}(\Lambda)$. By assumptions the set of such vectors f is dense in the space H.

Analogously, for the right-hand side of (5.14)

$$\left(A_0^{-1} + \Pi(\Pi^* B\Pi)^{-1}\Pi^*\right) f = \left(A_0^{-1} + \Pi(\Pi^* B\Pi)^{-1}\Pi^*\right)(f_\perp + B\Pi\varphi) = u$$

where $u = A_0^{-1}(f_\perp + B\Pi\varphi) + \Pi\varphi$. Application of L_B defined in (5.13) to both sides gives the desired result (here $h = \Pi\varphi$):

$$\begin{aligned} L_B\left(A_0^{-1} + \Pi(\Pi^* B\Pi)^{-1}\Pi^*\right) f &= L_B\left(A_0^{-1}(f_\perp + B\Pi\varphi) + \Pi\varphi\right) \\ &= f_\perp + B\Pi\varphi \\ &= f. \end{aligned}$$

The formula $L_B^{-1} = A_0^{-1} + \Pi(\Pi^* B\Pi)^{-1}\Pi^*$ now follows from the usual density arguments.

Considering operator-function $Q(z) = Q_{\beta_0,\beta_1}(z)$ with $\beta_0 = \Lambda + \Pi^* B\Pi$ and $\beta_1 = -I$,

$$Q(z) = -(\overline{\beta_0 + \beta_1 M(z)})^{-1}\beta_1 = (\overline{\Lambda + \Pi^* B\Pi - M(z)})^{-1} = -(M_B(z))^{-1}.$$

Since $Q(0) = -(M_B(0))^{-1} = -\Lambda_B^{-1} = (\Pi B\Pi^*)^{-1}$ is bounded by assumption, operators $Q_{\beta_0,\beta_1}(z)$ exist and are bounded at least for small $|z|$. According to Theorem 5.1 and representation (5.1) (see Corollary 5.1) the inverse $(A_{\beta_0,\beta_1})^{-1}$ is bounded and

$$(A_{\beta_0,\beta_1})^{-1} = A_0^{-1} + \Pi Q(0)\Pi^* = A_0^{-1} - \Pi\Lambda_B^{-1}\Pi^* = A_0^{-1} + \Pi(\Pi^* B\Pi)^{-1}\Pi^*,$$

which coincides with L_B^{-1}. The last assertion again follows from Theorem 5.1. □

Simple corollaries of Theorem 5.3 and definition of L_B are given below. Their consequences will not be pursued here, see [71, 73] for further details.

Remark 5.5. Statements of Theorem 5.3 can be used to describe dependence of M-operator on the particular choice of Λ in Definition 3.3 of boundary operator Γ_1. Obviously, if $B = B^*$ and the operator Γ_1 is defined with Λ replaced by Λ_B, i.e., as $\Gamma_1 : A_0^{-1} f + \Pi\varphi \mapsto \Pi^* f + \Lambda_B\varphi$ for $f \in H$, $\varphi \in \mathcal{D}(\Lambda)$, then all results remain valid with L_B playing the role of operator A_1 with $M_B(z)$ being the M-function.

Remark 5.6. The equality $\Lambda = \Lambda_B$ is only possible if

$$\Gamma_1(I + A_0^{-1}B)\Pi\varphi = 0, \quad \varphi \in \mathcal{D}(\Lambda)$$

by virtue of representations $\Lambda = \Gamma_1\Pi$ and $\Lambda_B = -\Pi^* B\Pi = -\Gamma_1 A_0^{-1} B\Pi$. It does not follow that the solution to this equation is $B = -A_0$. In fact, this equality contradicts the assumption $\mathcal{D}(B) \supset \Pi\mathcal{D}(\Lambda)$ about operator B since $\mathcal{D}(A_0) \cap \mathcal{R}(\Pi) = \{0\}$. When B is such that $\Lambda = \Lambda_B$ then L_B and A_1 coincide due to Corollary 5.3 *(*or the equalities $\beta_1 = -I$, $\beta_0 = 0$ that follow from Theorem 5.3*)*.

Remark 5.7. The operator A_K corresponding to $B = 0$ is an analogue of Krein's extension of A_{00} characterized by the boundary condition $(\Gamma_1 - \Lambda\Gamma_0)u = 0$ see [6, 35, 36, 44]. Note that the semiboundedness of A_{00} is not required for this definition of Krein's extension *(*cf. [38]*)*. The formal equality $B = \infty$ corresponds to the operator $L_B = A_0$.

6. Cayley Transform of M-function. Applications to the scattering theory

This section outlines basic results on the scattering theory for operators corresponding to boundary conditions studied in the previous section. In order to investigate selfadjoint and nonselfadjoint cases simultaneously the schema based on the functional model for linear operators suggested by S. Naboko in papers [60, 61] is proposed. The central ingredient of this schema is a dissipative operator whose B. Sz.-Nagy and C. Foias functional model [62] serves as the model space for all operators under consideration. Papers [60, 61] are devoted to the case of additive perturbations of a selfadjoint operator and offer an explicit form for the "model" dissipative operator used in the study. The crucial element of the approach is availability of a certain factorization of the perturbation which allows the subsequent model construction. These assumptions regarding perturbations render the schema of [60, 61] not applicable to linear operators associated with boundary value problems because they can not be represented as additive perturbations of one another. The obvious way to circumvent this difficulty, at least in case of elliptic boundary value problems, is to investigate inverse operators instead of the "direct" ones [12]. Since the inverses are bounded, their differences are well defined bounded operators, and the method of [60, 61] is fully applicable provided the "model" dissipative operator is suitably chosen. This chapter suggests such an operator based on considerations involving the Cayley transform of M-function. In addition, the required factorizations turn out to be direct consequences of formulas of previous section, see especially Corollary 5.1. Necessary connections to the theory of dissipative operators and functional models are established by the relationship between the M-function and the so-called characteristic function of a "minimal" symmetric operator discussed in papers [24, 42, 43, 79] in other contexts. The exposition in this section is carried out in the spirit of nonselfadjoint operator theory and concludes with a brief sketch illustrating the proposed approach in Remark 6.3.

It is convenient to begin with the following observation. Since values of $M(z)$, $z \in \mathbb{C}_+$ are (possibly unbounded) operators with positive imaginary part, operators $M(z) + iI$ are boundedly invertible for $z \in \mathbb{C}_+$. Moreover, a short argument shows that the Cayley transform of $M(z)$ defined as $\Theta(z) = (M(z) - iI)(M(z) + iI)^{-1}$ is analytic and contractive for $z \in \mathbb{C}_+$. It turns out that $\Theta(z)$ for $z \in \mathbb{C}_+$ is the characteristic function of some dissipative operator L in the sense of A. Štraus [78]. This fact was first observed in [42, 43, 79] for the characteristic function of Cayley transform of A_{00} extended by the null map on $[\mathcal{R}(A_{00}+iI)]^\perp$ to the partial isometry defined everywhere in H, and then reformulated in the setting of boundary triplets (under assumptions $\mathcal{R}(\Gamma_0) = \mathcal{R}(\Gamma_1) = E$ and $M(z)$ bounded) for the characteristic function of respective dissipative operator in [24]. The following Theorem renders these results in the form convenient for the discussion of nonselfadjoint scattering theory at the end of this section. Note that boundedness of $M(z)$ below is not required.

Theorem 6.1. *Operator L defined by the boundary condition* $(\Gamma_1 - i\Gamma_0)u = 0$ *according to the Theorem* 5.1 *with* $\beta_0 = -iI$, $\beta_1 = I$ *is dissipative and boundedly invertible. The inverse of L is the operator* $T = A_0^{-1} - \Pi(\Lambda - iI)^{-1}\Pi^*$. *For* $z \in \mathbb{C}_+$ *the characteristic function of L is given by the formula:*

$$\Theta(z) = (\Lambda - iI)(\Lambda + iI)^{-1} + 2iz(\Lambda + iI)^{-1}\Pi^*(I - zT^*)^{-1}\Pi(\Lambda + iI)^{-1}.$$

For $z \in \mathbb{C}_+$ *this function coincides with the Cayley transform of* $M(z)$,

$$\Theta(z) = (M(z) - iI)(M(z) + iI)^{-1}, \quad z \in \mathbb{C}_+.$$

Before turning to the proof, let us recall the definition of characteristic function of L according to [78]. This definition is equivalent to the definition given by M. Livšic [50] and independently by B. Sz.-Nagy and C. Foias [62] and has been proven more convenient in practical applications.

Following [78], introduce a sesquilinear form $\Psi(\cdot,\cdot)$ defined on the domain $\mathcal{D}(L) \times \mathcal{D}(L)$:

$$\Psi(u, v) = \frac{1}{2i}[(Lu, v)_H - (u, Lv)_H], \quad u, v \in \mathcal{D}(L),$$

and a linear set $\mathcal{G}(L) = \{v \in \mathcal{D}(L) \mid \Psi(u, v) = 0, \forall v \in \mathcal{D}(L)\}$. Define the linear space $\mathfrak{L}(L)$ as a closure of the quotient space $\mathcal{D}(L)/\mathcal{G}(L)$ endowed with the inner product $[\xi, \eta]_{\mathfrak{L}} = \Psi(f, g)$, where $\xi, \eta \in \mathfrak{L}(L)$ and $u \in \xi$, $v \in \eta$. Obviously, $\mathfrak{L}(L) = \{0\}$ if L is symmetric. A *boundary space* for the operator L is any linear space $\mathfrak{L}$ which is isomorphic to $\mathfrak{L}(L)$. A *boundary operator* for the operator L is the linear map Γ with the domain $\mathcal{D}(L)$ and the range in the boundary space $\mathfrak{L}$ such that

$$[\Gamma u, \Gamma v]_{\mathfrak{L}} = \Psi(u, v), \quad u, v \in \mathcal{D}(L).$$

Let $\mathfrak{L}'$ with the inner product $[\cdot,\cdot]'$ be a boundary space for $-L^*$ with the boundary operator Γ' mapping $\mathcal{D}(L^*)$ onto $\mathfrak{L}'$. A *characteristic function* of the operator L is an operator-valued function θ defined on the set $\rho(L^*)$ whose values $\theta(z)$ map $\mathfrak{L}$ into $\mathfrak{L}'$ according to the equality

$$\theta(z)\Gamma u = \Gamma'(L^* - zI)^{-1}(L - zI)u, \quad u \in \mathcal{D}(L).$$

Since the right-hand side of this formula is analytic with regard to $z \in \rho(L^*)$, the function θ is analytic on $\rho(L^*)$.

This construction needs to be applied to the operator L from Theorem 6.1 defined by the boundary condition $(\Gamma_1 - i\Gamma_0)u = 0$. To that end, notice that $\beta_0 = -iI$ and $\beta_1 = I$, and therefore $\mathscr{B} = \beta_0 + \beta_1\Lambda = -iI + \Lambda$ is boundedly invertible as $\Lambda = \Lambda^*$. The operator function $Q(z) = -\overline{(\beta_0 + \beta_1 M(z))}^{-1}\beta_1$ has the representation $Q(z) = -(M(z) - iI)^{-1}$ and is bounded for $z \in \mathbb{C}_-$. In accordance with Theorem 5.1 and Corollary 5.1, the inverse L^{-1} exists and

$$L^{-1} = A_0^{-1} + \Pi Q(0)\Pi^* = A_0^{-1} - \Pi(\Lambda - iI)^{-1}\Pi^*.$$

Denote $T = L^{-1}$ and compute the imaginary part of T defined as $\mathrm{Im}\,(T) = (T - T^*)/2i$. We have

$$\begin{aligned} T - T^* = L^{-1} - (L^{-1})^* &= -\Pi(\Lambda - iI)^{-1}\Pi^* + \Pi(\Lambda + iI)^{-1}\Pi^* \\ &= \Pi(\Lambda + iI)^{-1}\left[(\Lambda - iI) - (\Lambda + iI)\right](\Lambda - iI)^{-1}\Pi^* \\ &= -2i\Pi(\Lambda + iI)^{-1}(\Lambda - iI)^{-1}\Pi^*. \end{aligned}$$

Therefore

$$\mathrm{Im}\,(T) = \frac{T - T^*}{2i} = -\Pi(\Lambda + iI)^{-1}(\Lambda - iI)^{-1}\Pi^*,$$

which shows that T^* is dissipative:

$$\mathrm{Im}\,(T^*) = \Pi(\Lambda + iI)^{-1}(\Lambda - iI)^{-1}\Pi^* \geq 0. \tag{6.1}$$

The proof of Theorem 6.1 is based on direct computations that closely follow the schema of A. Štraus [78].

Proof. Suppose $u, v \in \mathcal{D}(L)$ and denote $Lu = f$, $Lv = g$. Then $f = Tu$, $g = Tv$ where $T = L^{-1}$ and for the form $\Psi(\cdot;\cdot)$ we have

$$\begin{aligned} \Psi(u,v) &= \frac{1}{2i}[(Lu,v) - (u,Lv)] = \frac{1}{2i}[(f,Tg) - (Tf,g)] \\ &= \left(\frac{T^* - T}{2i}f, g\right) = (\mathrm{Im}\,(T^*)f, g) \\ &= ((\Lambda - iI)^{-1}\Pi^* f, (\Lambda - iI)^{-1}\Pi^* g) = ((\Lambda - iI)^{-1}\Pi^* Lu, (\Lambda - iI)^{-1}\Pi^* Lv). \end{aligned}$$

Thus, the boundary space $\mathfrak{L}$ for L can be chosen as a closure of $\mathcal{R}((\Lambda - iI)^{-1}\Pi^*)$ with the boundary operator $\Gamma = (\Lambda - iI)^{-1}\Pi^* L$:

$$\mathfrak{L} = \overline{\mathcal{R}((\Lambda - iI)^{-1}\Pi^* L)}, \quad \Gamma : u \mapsto (\Lambda - iI)^{-1}\Pi^* Lu, \quad u \in \mathcal{D}(L).$$

Note that the metric in $\mathfrak{L}$ is positive definite, and $\mathfrak{L}$ is in fact a Hilbert space. Analogous computations for $(-L^*)$ justify the following choice of boundary space $\mathfrak{L}'$ and boundary operator Γ'

$$\mathfrak{L}' = \overline{\mathcal{R}((\Lambda + iI)^{-1}\Pi^* L^*)}, \quad \Gamma' : v \mapsto (\Lambda + iI)^{-1}\Pi^* L^* v, \quad v \in \mathcal{D}(L^*).$$

Here $\mathfrak{L}'$ is a Hilbert space.

In order to calculate the characteristic function $\Theta(z)$ of operator L corresponding to this choice of boundary spaces and operators, set again $u = Tf$ with

$f \in H$ so that $f = Lu$. For $z \in \rho(L^*)$ we have

$$\begin{aligned}
&\Gamma'(L^* - zI)^{-1}(L - zI)u \\
&\qquad = (\Lambda + iI)^{-1}\Pi^* L^*(L^* - zI)^{-1}(L - zI)L^{-1}f \\
&\qquad = (\Lambda + iI)^{-1}\Pi^*(I - zT^*)^{-1}(I - zT)f \\
&\qquad = (\Lambda + iI)^{-1}\Pi^*(I - zT^*)^{-1}(I - zT^* + z(T^* - T))f \\
&\qquad = (\Lambda + iI)^{-1}\Pi^*\left[I + 2iz(I - zT^*)^{-1}(\mathrm{Im}\,(T^*))\right] f \\
&\qquad = (\Lambda + iI)^{-1}\Pi^*\left[I + 2iz(I - zT^*)^{-1}\Pi(\Lambda + iI)^{-1}(\Lambda - iI)^{-1}\Pi^* f\right] \\
&\qquad = \left[(\Lambda - iI)(\Lambda + iI)^{-1} + 2iz(\Lambda + iI)^{-1}\Pi^*(I - zT^*)^{-1}\Pi(\Lambda + iI)^{-1}\right] \\
&\qquad\quad \times (\Lambda - iI)^{-1}\Pi^* f.
\end{aligned}$$

Since $(\Lambda - iI)^{-1}\Pi^* f = (\Lambda - iI)^{-1}\Pi^* Lu = \Gamma u$, this formula shows that the characteristic function of L coincides with the expression in brackets, that is, the function $\Theta(z)$ from the Theorem statement.

For the verification of identity $\Theta = (M - iI)(M + iI)^{-1}$ write down the adjoint of function Θ

$$[\Theta(\bar{z})]^* = (\Lambda + iI)(\Lambda - iI)^{-1} - 2iz(\Lambda - iI)^{-1}\Pi^*(I - zT)^{-1}\Pi(\Lambda - iI)^{-1}, \quad z \in \mathbb{C}_-.$$

By virtue of equality $Q(0) = -(\Lambda - iI)^{-1}$ and Corollary 5.1,

$$\begin{aligned}
z(\Lambda - iI)^{-1}\Pi^*(I - zT)^{-1}\Pi(\Lambda - iI)^{-1} &= zQ(0)\Pi^*(I - zL^{-1})^{-1}\Pi Q(0) \\
&= Q(z) - Q(0) \\
&= -(M(z) - iI)^{-1} + (\Lambda - iI)^{-1}
\end{aligned}$$

Therefore

$$\begin{aligned}
[\Theta(\bar{z})]^* &= (\Lambda + iI)(\Lambda - iI)^{-1} + 2i(M(z) - iI)^{-1} - 2i(\Lambda - iI)^{-1} \\
&= I + 2i(M(z) - iI)^{-1} = (M(z) + iI)(M(z) - iI)^{-1}.
\end{aligned}$$

By passing to the adjoint operators and noticing that $[M(\bar{z})]^* = M(z)$ the claimed identity follows. □

Remark 6.1. The characteristic function of a linear operator is not determined uniquely [13, 62, 78]. Namely, consider two isometries $\tau : \mathfrak{L} \to \widetilde{\mathfrak{L}}$ and $\tau' : \mathfrak{L}' \to \widetilde{\mathfrak{L}}'$ of the boundary spaces $\mathfrak{L}$, $\mathfrak{L}'$ of operator L to another pair of spaces $\widetilde{\mathfrak{L}}$, $\widetilde{\mathfrak{L}}'$. It is easy to see that the characteristic function of L corresponding to the pair $\widetilde{\mathfrak{L}}$, $\widetilde{\mathfrak{L}}'$ is the function $\widetilde{\theta}(z) = \tau'\theta(z)\tau^*$. In application to the characteristic function $\Theta(z)$ above observe that the operator $U = (\Lambda - iI)(\Lambda + iI)^{-1}$ is an unitary in E. Therefore, both functions $U^*\Theta(z)$ and $\Theta(z)U^*$, $z \in \mathbb{C}_+$

$$\begin{aligned}
U^*\Theta(z) &= I + 2iz(\Lambda - iI)^{-1}\Pi^*(I - zT^*)^{-1}\Pi(\Lambda + iI)^{-1}, \\
\Theta(z)U^* &= I + 2iz(\Lambda + iI)^{-1}\Pi^*(I - zT^*)^{-1}\Pi(\Lambda - iI)^{-1}
\end{aligned}$$

are characteristic functions of L, although corresponding to alternative choices of boundary spaces and operators.

Remark 6.2. Direct calculations as outlined above yield the following expression for the characteristic function $\vartheta(z)$ of dissipative operator $T^* = (L^*)^{-1}$:

$$\vartheta(\zeta) = I + 2i(\Lambda + iI)^{-1}\Pi^*(T - \zeta I)^{-1}\Pi(\Lambda - iI)^{-1}, \quad \zeta \in \mathbb{C}_+.$$

By virtue of (6.1) this characteristic function is given in its "standard" form, which is consistent with the expression for characteristic function $W(z) = I + 2iK^*(A^* - zI)^{-1}K$ of a bounded dissipative operator $A = R + iQ$ with $R = R^*$, $Q = Q^* \geq 0$ and $Q = KK^*$ *(*or the corresponding operator node*)* that can be found in the literature [13, 62]. A close relationship between $\vartheta(\zeta)$ and $\Theta(z)$ is clarified by the substitution $\zeta \to z = 1/\zeta$

$$\vartheta(1/z) = I - 2iz(\Lambda + iI)^{-1}\Pi^*(I - zT)^{-1}\Pi(\Lambda - iI)^{-1}, \quad z \in \mathbb{C}_-.$$

Comparison with the expression for the adjoint of $[\Theta(\bar{z})U^*]$ leads to the identity

$$\vartheta(1/z) = U\,[\Theta(\bar{z})]^*\,, \quad z \in \mathbb{C}_-$$

where $U = (\Lambda - iI)(\Lambda + iI)^{-1}$ is an unitary.

Remark 6.3. Dissipative operator $T^* = (L^{-1})^* = A_0^{-1} - \Pi(\Lambda + iI)^{-1}\Pi^*$ can be employed for the development of scattering theory of *(*in general, nonselfadjoint*)* operators $L^\varkappa$ defined by boundary conditions $(\Gamma_1 + \varkappa\Gamma_0)u = 0$ with $\varkappa : E \to E$. Assume $\Lambda + \varkappa$ is boundedly invertible. Then the inverse $T_\varkappa = (L^\varkappa)^{-1}$ exists and $T_\varkappa = A_0^{-1} - \Pi(\Lambda + \varkappa)^{-1}\Pi^*$ by Corollary 5.1. The functional model construction for additive perturbations [60] is fully applicable to A_0^{-1}, T^*, $T_\varkappa$, which makes possible development of the scattering theory for A_0^{-1} and $T_\varkappa$. Application of the invariance principle for the function $t \to (1/t)$, $t \in \mathbb{R}$, $t \neq 0$ yields existence and completeness results for the local wave operators for the pairs $(A_0, L^\varkappa)$, and $(L^\varkappa, A_0)$. The interested reader is referred to the works [60, 61, 69, 72] for further details on the functional model of nonselfadjoint operators and its applications to the scattering theory.

7. Singular Perturbations

The schema developed in preceding sections is essentially axiomatic. The only condition imposed on the set $\{A_0^{-1}, \Pi, \Lambda\}$ is the validity of two Assumptions from Sect. 3, whereas nothing specific is requested of the "boundary". Due to this fact, our approach is applicable in situations not readily covered by the traditional boundary problems technique. For instance, it makes possible a construction of "boundary value problem" when no boundary is given a priori. Introduction of an artificial boundary is a certain form of perturbation that is not "regular" in the traditional sense. Such "singular" perturbations are typical in the open systems theory where they are identified with the open channels connecting the system with its environment [51]. From this point of view, the selfadjoint operator A_0 acting in the "inner space" H describes the "unperturbed system" coupled with the "external space" E by means of the "channel" operator $\Pi : E \to H$. The "coupling" takes place at the "boundary". More details on connections to the open systems theory can be found in [73].

This section offers an illustration of these ideas by means of an elementary example considered previously within the framework of boundary triples in [70]. We study the physical model of a quantum particle in the potential field of finite number of singular interactions modeled by Dirac's δ-functions. The free particle is described by the Hamiltonian operator which in this case is the "free" Laplacian acting in $L^2(\mathbb{R}^3)$, and the point interactions define "perturbations" of the unperturbed system (see [3, 4, 5] and references therein). Within the paper's context, the points where the interactions are situated form the "boundary" of the "boundary value problem."

Let $H := L^2(\mathbb{R}^3)$. Denote A_0 the selfadjoint boundedly invertible operator $I-\Delta$ in H with domain $\mathcal{D}(A_0) := H^2(\mathbb{R}^3)$. The fundamental solution to the equation $((I-\Delta)-zI)u = 0$, $z \in \mathbb{C}\setminus[1,\infty)$ is the square summable function $\mathscr{G}_z(x) = \frac{1}{4\pi}\frac{\exp(i\sqrt{z-1}|x|)}{|x|}$. Fix a finite set of distinct points $x_j \in \mathbb{R}^3$, $j = 1, 2, \dots, n$ and introduce n functions $\mathcal{G}_j(x,z) := \mathscr{G}_z(x-x_j)$. Formally, each $\mathcal{G}_j(x,z)$ is the solution to the partial differential equation $((I-\Delta)-zI)u = \delta(x-x_j)$. Any function $\mathcal{G}_j(x,z)$ is infinitely differentiable in any domain that does not contain x_j. Because of the singularity at $x \to x_j$ functions $\mathcal{G}_j(x,z)$ are not in $\mathcal{D}(A_0)$. However, for any $z, \zeta \in \mathbb{C}\setminus[1,\infty)$ the difference $\mathcal{G}_j(x,z) - \mathcal{G}_j(x,\zeta)$ lies in $\mathcal{D}(A_0)$. In the following the abridged notation $\mathcal{G}_j$ for $\mathcal{G}_j(x,0)$ will be used. Notice that $\mathcal{G}_j$ are linearly independent as elements of $H = L_2(\mathbb{R}^3)$.

Choose the space E to be the n-dimensional Euclidian $E = \mathbb{C}^n$ with the orthonormal basis $\{e_j\}_1^n$ and define the operator $\Pi : E \to H$ on $\{e_j\}_1^n$ by $\Pi : e_j \mapsto \mathcal{G}_j$. It follows that $\Pi : a \mapsto \sum a_j\mathcal{G}_j$ where $a = \sum a_j e_j$ is an element of E. Since $\mathcal{R}(\Pi)\cap\mathcal{D}(A_0) = \{0\}$ and the inverse to Π is the mapping $\sum a_j\mathcal{G}_j \mapsto \{a_j\}_{j=1}^n$, Assumption 1 holds. Therefore we can introduce the operator A on domain $\mathcal{D}(A) := \mathcal{D}(A_0)\dot{+}\mathcal{H}$, where $\mathcal{H} := \mathcal{R}(\Pi) = \bigvee \mathcal{G}_j$. According to the Sect. 3, $A : A_0^{-1}f + \sum a_j\mathcal{G}_j \mapsto f$, $f \in H$. The equality $\operatorname{Ker}(A) = \mathcal{H}$ can be understood literally, because $(I-\Delta)\mathcal{G}_j = \delta(x-x_j)$ and the right hand side is supported on the set of zero Lebesgue measure in $\mathbb{R}^3$. Further, the boundary operator Γ_0 defined on $\mathcal{D}(\Gamma_0) = \mathcal{D}(A)$ acts according to the rule $\Gamma_0 : f_0 + \sum a_j\mathcal{G}_j \mapsto \{a_j\}_1^n$, where $f_0 \in \mathcal{D}(A_0)$ and $\{a_j\}_1^n \in E$. Due to identity $\Gamma_0\mathcal{G}_j = e_j$ we have $\operatorname{Ker}(\Gamma_0) = \mathcal{D}(A_0)$. The requirements $\Gamma_0\Pi = I_E$ and $\Pi\Gamma_0\mathcal{G}_j = \mathcal{G}_j$ therefore are met.

The operator S_z maps $a \in E$ into a unique solution u_z of the equation $(A-zI)u = 0$ satisfying condition $\Gamma_0 u = a$. It is not difficult to see that S_z has the form

$$S_z : \{a_j\}_1^n \mapsto u_z = \sum_j a_j\mathcal{G}_j(x,z), \quad z \in \mathbb{C}_\pm.$$

Indeed, the fact $\mathcal{G}_j(x,z) \in \operatorname{Ker}(A - zI)$ was discussed above, and the boundary condition is verified by direct computations. For $a = \sum_j a_j e_j$ we have

$$\Gamma_0 S_z a = \sum_j a_j \Gamma_0 \mathcal{G}_j(x,z) = \sum_j a_j \Gamma_0 \mathcal{G}_j + \sum_j a_j \Gamma_0 \left(\mathcal{G}_j(x,z) - \mathcal{G}_j\right) = \sum_j a_j e_j = a$$

because $\Gamma_0 \mathcal{G}_j = I$ and the difference $\mathcal{G}_j(x,z) - \mathcal{G}_j$ belongs to $\mathcal{D}(A_0)$, therefore to $\operatorname{Ker}(\Gamma_0)$.

To calculate the adjoint $\Pi^* : H \to E$ and choose the operator Λ in the representation $\Gamma_1 = \Pi^* A + \Lambda \Gamma_0$ appropriately suppose $a = \sum a_j e_j$ and $f \in H$. Then $(\Pi a, f) = \sum a_j (\mathcal{G}_j, f) = \langle a, \sum (f, \mathcal{G}_j) e_j \rangle$, hence Π^* is defined as $\Pi^* : f \mapsto \sum (f, \mathcal{G}_j) e_j$. If $f = A_0 f_0$ with some $f_0 \in \mathcal{D}(A_0)$, then $\Pi^* A f_0 = \Pi^* A_0 f_0 = \sum (A_0 f_0, \mathcal{G}_j) e_j$. Summands here are easy to compute. It follows from the properties of fundamental solutions $\mathcal{G}_j$ that $(A_0 f_0, \mathcal{G}_j) = f_0(x_j)$, therefore $\Gamma_1|_{\mathcal{D}(A_0)} = \Pi^* A_0 : f_0 \mapsto \sum f_0(x_j) e_j$ for $f_0 \in \mathcal{D}(A_0)$.

The operator Λ describing Γ_1 restricted to the set $\mathcal{R}(\Pi)$ can be chosen arbitrarily as long as it is selfadjoint. For example, it could be taken as the identity $\Lambda = I_E$ or the null operator $\Lambda : a \mapsto 0$, $a \in E$. However, it is convenient to define the action of Γ_1 on $\mathcal{R}(\Pi)$ consistently with its action on $\mathcal{D}(A_0)$. Since $\Gamma_1|_{\mathcal{D}(A_0)}$ evaluates functions $f_0 \in \mathcal{D}(A_0)$ at the points $\{x_j\}_1^n$ and then builds a corresponding vector $\{f_0(x_j)\}_1^n$ in $E = \mathbb{C}^n$, we would like $\Gamma_1|_{\mathcal{R}(\Pi)}$ to act similarly. Functions $\mathcal{G}_j(x)$ are easily evaluated at x_s for $s \neq j$, but $\mathcal{G}_j$ is not defined at $x = x_j$; thus is not possible to define Γ_1 on $\mathcal{R}(\Pi) = \bigvee \mathcal{G}_j$ to be the evaluation operator. To circumvent this problem recall that in the neighborhood of x_j the function $\mathscr{G}_z(x - x_j)$ has the following asymptotic expansion

$$\begin{aligned}\mathscr{G}_z(x - x_j) &= \frac{1}{4\pi} \frac{\exp\left(i\sqrt{z-1}|x - x_j|\right)}{|x - x_j|} \\ &\sim \frac{1}{4\pi}\left(\frac{1}{|x - x_j|} + i\sqrt{z-1} + O(|x - x_j|)\right).\end{aligned}$$

Define the action Γ_1 on the vector $\mathscr{G}_z(x - x_j)$ as

$$\Gamma_1 : \mathscr{G}_z(x - x_j) \mapsto \frac{i\sqrt{z-1}}{4\pi} e_j + \sum_{s \neq j} \mathscr{G}_z(x_j - x_s) e_s$$

where $\frac{i\sqrt{z-1}}{4\pi}$ is the coefficient in the asymptotic expansion above corresponding to $|x - x_j|$ to the power 0. In particular, for $z = 0$,

$$\Gamma_1 : \mathcal{G}_j \mapsto -\frac{1}{4\pi} e_j + \sum_{s \neq j} \mathcal{G}_j\big|_{x = x_s} e_s$$

where $\mathcal{G}_j\big|_{x = x_s} = \mathcal{G}_j(x_s, 0) = \mathscr{G}_0(x_j - x_s)$, $s \neq j$. Thus for $a = \{a_j\}_1^n \in E$,

$$\Gamma_1 : \Pi a = \sum_j a_j \mathcal{G}_j \mapsto \left\{ -a_j \frac{1}{4\pi} + \sum_{s \neq j} a_s \mathcal{G}_s\big|_{x = x_j} \right\}_{j=1}^n.$$

The next step is the calculation of M-operator of A. Quite analogously to the computation of $\Gamma_1\Pi$ above we have for $a = \{a_j\}_1^n = \sum_j a_j e_j \in E$,

$$\Gamma_1 : \sum_j a_j \mathcal{G}_j(x,z) \mapsto \left\{ a_j \frac{i\sqrt{z-1}}{4\pi} + \sum_{s\neq j} a_s\ \mathcal{G}_s(x_j,z) \right\}_{j=1}^n .$$

Since $S_z a = \sum_j a_j \mathcal{G}_j(x,z)$, this formula yields for $M(z)a = \Gamma_1 S_z a$,

$$\begin{aligned} M(z)a &= \Gamma_1 \left(\sum_j a_j \mathcal{G}_j(x,z) \right) \\ &= \frac{1}{4\pi} \left\{ i a_j \sqrt{z-1} + \sum_{s\neq j} a_s \frac{\exp\left(i\sqrt{z-1}|x_j - x_s|\right)}{|x_j - x_s|} \right\}_{j=1}^n . \end{aligned}$$

Therefore the operator-function $M(z)$ is the $n\times n$-matrix function with elements

$$M_{js}(z) = \frac{1}{4\pi} \begin{cases} i\sqrt{z-1}\,, & j = s, \\ \frac{\exp\left(i\sqrt{z-1}\,|x_j - x_s|\right)}{|x_j - x_s|}\,, & j \neq s. \end{cases}$$

By the change of variable $z \mapsto z+1$ the matrix $M(z+1)$ can be interpreted as the M-function of the Laplacian $-\Delta = A - I$ in $L_2(\mathbb{R}^3)$ perturbed by a set of point interactions $\{\delta(x-x_j)\}_1^n$. To elaborate more on this statement consider extensions of symmetric operator A_{00} defined as $-\Delta + I$ on the domain

$$\mathcal{D}(A_{00}) = \{u \in \mathcal{D}(A_0) \mid \Gamma_1 u = 0\} = \big\{u \in H^2(\mathbb{R}^3) \mid u(x_s) = 0,\ s = 1,2,\ldots,n\big\}.$$

Suppose the operator A^β is defined as a restriction of A to domain

$$\mathcal{D}(A^\beta) = \{u \in \mathcal{D}(A) \mid (\beta_0\Gamma_0 + \beta_1\Gamma_1)u = 0\}$$

where β_0, β_1 are arbitrary $n\times n$-matrices. The resolvent of A^β is described in Theorem 5.1. In particular, assuming that $\beta_0 + \beta_1\Lambda$ where $\Lambda = M(0)$ is boundedly invertible, the inverse of A^β as given by Corollary 5.1 is

$$(A^\beta)^{-1} = A_0^{-1} - \Pi(\beta_0 + \beta_1\Lambda)^{-1}\beta_1\Pi^*. \tag{7.1}$$

Consider sesquilinear forms of both sides of this identity on a pair of vectors $f, g \in H$. Since $\mathcal{R}(A_0) = H$, vectors f and g can be represented as $f = A_0 u$, $g = A_0 v$ with some $u, v \in \mathcal{D}(A_0)$. Then the form on the right is

$$(A_0^{-1}f, g) - (\Pi(\beta_0 + \beta_1\Lambda)^{-1}\beta_1\Pi^* f, g) = (A_0 u, v) - ((\beta_0 + \beta_1\Lambda)^{-1}\beta_1\Gamma_1 u, \Gamma_1 v),$$

due to equalities $\Pi^* f = \Gamma_1 A_0^{-1} A_0 u = \Gamma_1 u$ and $\Pi^* g = \Gamma_1 v$. Notice that vectors $\Gamma_1 u$ and $\Gamma_1 v$ are known explicitly, namely $\Gamma_1 u = \{u(x_j)\}_1^n$ and $\Gamma_1 v = \{v(x_j)\}_1^n$.

In order to clarify meaning of the form $((A^\beta)^{-1}f, g)$ of the operator on the left hand side of (7.1) we need to recall some basic concepts from the theory of scales of Hilbert spaces [10]. Introduce the rigging $H^+ \subset H \subset H^-$ of H constructed by the positive boundedly invertible operator $A_0 = -\Delta + I$. The positive space H^+ consists of elements from $\mathcal{D}(A_0)$ and is equipped with the norm $\|u\|_+ = \|A_0 u\|_H$, $u \in \mathcal{D}(A_0)$. It follows that A_0 acts as an isometry from H^+ onto H. The dual space H^- is identified with the Hilbert space of all antilinear functionals over elements from H^+ with respect to the inner product in H. In the usual way, the product $(f,g)_H$ of two vectors $f,g \in H$ is naturally extended to the duality relation between $f \in H^-$ and $g \in H^+$. This construction allows one to consider a continuation A_0^+ of A_0 from the domain $\mathcal{D}(A_0)$ to the whole of H. The map A_0^+ is defined on H by the formula $(A_0^+ f, v) = (f, A_0 v)$, $f \in H$, $v \in H^+$ and its range coincides with H^-. The sesquilinear form of $(A^\beta)^{-1}$ on the left hand side of (7.1) calculated on the pair $A_0 u, A_0 v$ now can be written as

$$((A^\beta)^{-1} A_0 u, A_0 v) = (A_0^+ (A^\beta)^{-1} A_0 u, v), \quad u, v \in H^+.$$

Thus the operator $\mathscr{A}^\beta := A_0^+ (A^\beta)^{-1} A_0$ acts from H^+ into H^- and its sesquilinear form is

$$(\mathscr{A}^\beta u, v) = (u, v) + (-\Delta u, v) + \sum_{j,k} \alpha_{jk} u(x_k) \overline{v(x_j)}, \quad u, v \in H^2(\mathbb{R}^3) \tag{7.2}$$

where α_{jk} are the matrix elements of the operator $-(\beta_0 + \beta_1 \Lambda)^{-1} \beta_1$ in the basis $\{e_j\}_1^n$.

Formula (7.2) relates ideas of this section to the conventional theory of point interactions. It is easily seen that the mapping $L^\beta = A_0^+ (A^\beta)^{-1} A_0$ is formally represented as $-\Delta + I + \alpha(\cdot\,, \vec{\delta})\,\vec{\delta}$ where $\vec{\delta} = \{\delta(x - x_j)\}_1^n$ and α is the matrix $\alpha = \|\alpha_{jk}\|$. Non-diagonal elements of α describe pairwise interactions between points $\{x_j\}$ themselves (the so called "non-local model" [46]), whereas the standard case of n mutually independent point interactions is recovered from (7.2) when the matrix α is diagonal. Under assumption $\beta_0 \beta_1^* = \beta_1 \beta_0^*$ the operator A^β is selfadjoint according to Corollary 5.2. Finally, Theorem 5.2 reduces the question of point spectrum of A^β to the study of $\det(\beta_0 + \beta_1 M(z))$, where $M(z)$ is the M-function discussed above. The point spectrum in the case $\beta_1 = I$ and the matrix β_0 diagonal was investigated in the work [82].

Notice in conclusion that considerations of this section suggest a consistent way to construct singular perturbations of differential operators by "potentials" supported by sets of Lebesgue measure zero in $\mathbb{R}^n$, cf. [3].

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This work is dedicated to the memory of Boris Pavlov (1936–2016), the role model of my academic career.

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