Operator Theory
Advances and Applications
232

Michael Demuth
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Mathematical Physics, Spectral Theory and Stochastic Analysis

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Contents

Preface

This volume contains survey articles on various aspects of operator theory and partial differential operators. These papers are meant as self-contained introductions to specific fields written by experts for non specialists. They are accessible for graduate students and young researchers but – we believe – they are also of interest to scientists already familiar with the respective area.

The topics covered range from differential operators on abstract manifolds to finite difference operators on a lattice modeling some aspects of impure superconductors. All of them share a view towards applications in physics.

The idea to collect these contributions arose during a conference organized by D. Mayer, I. Witt and one of the editors in Goslar (Germany) in September 2011. But, instead of collecting highly specialized articles on most recent research as for conference proceedings our focus was on introductory aspects and readability of up-to-date contributions.

During the Goslar conference mentioned we also had the opportunity to celebrate the 65th birthday of Michael Demuth. It gives me a great pleasure to wish him here once more many happy years to come.

October 2012

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A Survey on the Krein–von Neumann Extension, the Corresponding Abstract Buckling Problem, and Weyl-type Spectral Asymptotics for Perturbed Krein Laplacians in Nonsmooth Domains

Mark S. Ashbaugh, Fritz Gesztesy, Marius Mitrea, Roman Shterenberg and Gerald Teschl

Dedicated with great pleasure to Michael Demuth on the occasion of his 65*th birthday*

Abstract. In the first (and abstract) part of this survey we prove the unitary equivalence of the inverse of the Krein–von Neumann extension (on the orthogonal complement of its kernel) of a densely defined, closed, strictly positive operator, $S \geq \varepsilon I_{\mathcal{H}}$ for some $\varepsilon > 0$ in a Hilbert space $\mathcal{H}$ to an abstract buckling problem operator.

In the concrete case where $S = \overline{-\Delta|_{C_0^\infty(\Omega)}}$ in $L^2(\Omega; d^n x)$ for $\Omega \subset \mathbb{R}^n$ an open, bounded (and sufficiently regular) set, this recovers, as a particular case of a general result due to G. Grubb, that the eigenvalue problem for the Krein Laplacian S_K (i.e., the Krein–von Neumann extension of S),

$$S_K v = \lambda v, \quad \lambda \neq 0,$$

is in one-to-one correspondence with the problem of *the buckling of a clamped plate*,

$$(-\Delta)^2 u = \lambda(-\Delta) u \text{ in } \Omega, \quad \lambda \neq 0, \quad u \in H_0^2(\Omega),$$

where u and v are related via the pair of formulas

$$u = S_F^{-1}(-\Delta) v, \quad v = \lambda^{-1}(-\Delta) u,$$

with S_F the Friedrichs extension of S.

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This establishes the Krein extension as a natural object in elasticity theory (in analogy to the Friedrichs extension, which found natural applications in quantum mechanics, elasticity, etc.).

In the second, and principal part of this survey, we study spectral properties for $H_{K,\Omega}$, the Krein–von Neumann extension of the perturbed Laplacian $-\Delta + V$ (in short, the perturbed Krein Laplacian) defined on $C_0^\infty(\Omega)$, where V is measurable, bounded and nonnegative, in a bounded open set $\Omega \subset \mathbb{R}^n$ belonging to a class of nonsmooth domains which contains all convex domains, along with all domains of class $C^{1,r}$, $r > 1/2$. (Contrary to other uses of the notion of "domain", a domain in this survey denotes an open set without any connectivity hypotheses. In addition, by a "smooth domain" we mean a domain with a sufficiently smooth, typically, a C^∞-smooth, boundary.) In particular, in the aforementioned context we establish the Weyl asymptotic formula

$$\#\{j \in \mathbb{N} \,|\, \lambda_{K,\Omega,j} \leq \lambda\} = (2\pi)^{-n} v_n |\Omega|\, \lambda^{n/2} + O\big(\lambda^{(n-(1/2))/2}\big) \text{ as } \lambda \to \infty,$$

where $v_n = \pi^{n/2}/\Gamma((n/2)+1)$ denotes the volume of the unit ball in $\mathbb{R}^n$, $|\Omega$ denotes the volume of Ω, and $\lambda_{K,\Omega,j}$, $j \in \mathbb{N}$, are the non-zero eigenvalues of $H_{K,\Omega}$, listed in increasing order according to their multiplicities. We prove this formula by showing that the perturbed Krein Laplacian (i.e., the Krein–von Neumann extension of $-\Delta + V$ defined on $C_0^\infty(\Omega)$) is spectrally equivalent to the buckling of a clamped plate problem, and using an abstract result of Kozlov from the mid 1980's. Our work builds on that of Grubb in the early 1980's, who has considered similar issues for elliptic operators in smooth domains, and shows that the question posed by Alonso and Simon in 1980 pertaining to the validity of the above Weyl asymptotic formula continues to have an affirmative answer in this nonsmooth setting.

We also study certain exterior-type domains $\Omega = \mathbb{R}^n \backslash K$, $n \geq 3$, with $K \subset \mathbb{R}^n$ compact and vanishing Bessel capacity $B_{2,2}(K) = 0$, to prove equality of Friedrichs and Krein Laplacians in $L^2(\Omega; d^n x)$, that is, $-\Delta|_{C_0^\infty(\Omega)}$ has a unique nonnegative self-adjoint extension in $L^2(\Omega; d^n x)$.

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Keywords. Lipschitz domains, Krein Laplacian, eigenvalues, spectral analysis, Weyl asymptotics, buckling problem.

Contents

1. Introduction

In connection with the first and abstract part of this survey, the connection between the Krein–von Neumann extension and an abstract buckling problem, suppose that S is a densely defined, symmetric, closed operator with nonzero deficiency indices in a separable complex Hilbert space $\mathcal{H}$ that satisfies

$$S \geq \varepsilon I_{\mathcal{H}} \text{ for some } \varepsilon > 0, \tag{1.1}$$

and denote by S_K and S_F the Krein–von Neumann and Friedrichs extensions of S, respectively (with $I_{\mathcal{H}}$ the identity operator in $\mathcal{H}$).

Then an abstract version of Proposition 1 in Grubb [97], describing an intimate connection between the nonzero eigenvalues of the Krein–von Neumann extension of an appropriate minimal elliptic differential operator of order $2m$,

$m \in \mathbb{N}$, and nonzero eigenvalues of a suitable higher-order buckling problem (cf. Example 3.5), to be proved in Lemma 3.1, can be summarized as follows:

$$\text{There exists } 0 \neq v \in \operatorname{dom}(S_K) \text{ satisfying } S_K v = \lambda v, \quad \lambda \neq 0, \tag{1.2}$$

if and only if

$$\text{there exists a } 0 \neq u \in \operatorname{dom}(S^*S) \text{ such that } S^*Su = \lambda Su, \tag{1.3}$$

and the solutions v of (1.2) are in one-to-one correspondence with the solutions u of (1.3) given by the pair of formulas

$$u = (S_F)^{-1} S_K v, \quad v = \lambda^{-1} Su. \tag{1.4}$$

Next, we will go a step further and describe a unitary equivalence result going beyond the connection between the eigenvalue problems (1.2) and (1.3): Given S, we introduce the following sesquilinear forms in $\mathcal{H}$,

$$a(u,v) = (Su, Sv)_{\mathcal{H}}, \quad u, v \in \operatorname{dom}(a) = \operatorname{dom}(S), \tag{1.5}$$

$$b(u,v) = (u, Sv)_{\mathcal{H}}, \quad u, v \in \operatorname{dom}(b) = \operatorname{dom}(S). \tag{1.6}$$

Then S being densely defined and closed, implies that the sesquilinear form a is also densely defined and closed, and thus one can introduce the Hilbert space

$$\mathcal{W} = (\operatorname{dom}(S), (\cdot,\cdot)_{\mathcal{W}}) \tag{1.7}$$

with associated scalar product

$$(u,v)_{\mathcal{W}} = a(u,v) = (Su, Sv)_{\mathcal{H}}, \quad u, v \in \operatorname{dom}(S). \tag{1.8}$$

Suppressing for simplicity the continuous embedding operator of $\mathcal{W}$ into $\mathcal{H}$, we now introduce the following operator T in $\mathcal{W}$ by

$$(w_1, Tw_2)_{\mathcal{W}} = a(w_1, Tw_2) = b(w_1, w_2) = (w_1, Sw_2)_{\mathcal{H}}, \quad w_1, w_2 \in \mathcal{W}. \tag{1.9}$$

One can prove that T is self-adjoint, nonnegative, and bounded and we will call T the *abstract buckling problem operator* associated with the Krein–von Neumann extension S_K of S.

Next, introducing the Hilbert space $\widehat{\mathcal{H}}$ by

$$\widehat{\mathcal{H}} = [\ker(S^*)]^{\perp} = \big[I_{\mathcal{H}} - P_{\ker(S^*)}\big]\mathcal{H} = \big[I_{\mathcal{H}} - P_{\ker(S_K)}\big]\mathcal{H} = [\ker(S_K)]^{\perp}, \tag{1.10}$$

where $P_{\mathcal{M}}$ denotes the orthogonal projection onto the subspace $\mathcal{M} \subset \mathcal{H}$, we introduce the operator

$$\widehat{S} : \begin{cases} \mathcal{W} \to \widehat{\mathcal{H}}, \\ w \mapsto Sw, \end{cases} \tag{1.11}$$

and note that $\widehat{S} \in \mathcal{B}(\mathcal{W}, \widehat{\mathcal{H}})$ maps $\mathcal{W}$ unitarily onto $\widehat{\mathcal{H}}$.

Finally, defining the *reduced Krein–von Neumann operator* $\widehat{S}_K$ in $\widehat{\mathcal{H}}$ by

$$\widehat{S}_K := S_K|_{[\ker(S_K)]^{\perp}} \text{ in } \widehat{\mathcal{H}}, \tag{1.12}$$

we can state the principal unitary equivalence result to be proved in Theorem 3.4:

The inverse of the reduced Krein–von Neumann operator $\widehat{S}_K$ in $\widehat{\mathcal{H}}$ and the abstract buckling problem operator T in $\mathcal{W}$ are unitarily equivalent,

$$\big(\widehat{S}_K\big)^{-1} = \widehat{S} T (\widehat{S})^{-1}. \tag{1.13}$$

In addition,

$$\big(\widehat{S}_K\big)^{-1} = U_S \big[|S|^{-1} S |S|^{-1}\big] (U_S)^{-1}. \tag{1.14}$$

Here we used the polar decomposition of S,

$$S = U_S|S|, \text{ with } |S| = (S^*S)^{1/2} \geq \varepsilon I_{\mathcal{H}}, \ \varepsilon > 0, \text{ and } U_S \in \mathcal{B}\big(\mathcal{H}, \widehat{\mathcal{H}}\big) \text{ unitary,} \tag{1.15}$$

and one observes that the operator $|S|^{-1}S|S|^{-1} \in \mathcal{B}(\mathcal{H})$ in (1.14) is self-adjoint in $\mathcal{H}$.

As discussed at the end of Section 4, one can readily rewrite the abstract linear pencil buckling eigenvalue problem (1.3), $S^*Su = \lambda Su$, $\lambda \neq 0$, in the form of the standard eigenvalue problem $|S|^{-1}S|S|^{-1}w = \lambda^{-1}w$, $\lambda \neq 0$, $w = |S|u$, and hence establish the connection between (1.2), (1.3) and (1.13), (1.14).

As mentioned in the abstract, the concrete case where S is given by $S = \overline{-\Delta|_{C_0^\infty(\Omega)}}$ in $L^2(\Omega; d^n x)$, then yields the spectral equivalence between the inverse of the reduced Krein–von Neumann extension $\widehat{S}_K$ of S and the problem of the buckling of a clamped plate. More generally, Grubb [97] actually treated the case where S is generated by an appropriate elliptic differential expression of order $2m$, $m \in \mathbb{N}$, and also introduced the higher-order analog of the buckling problem; we briefly summarize this in Example 3.5.

The results of this connection between an abstract buckling problem and the Krein–von Neumann extension in Section 3 originally appeared in [30].

Turning to the second and principal part of this survey, the Weyl-type spectral asymptotics for perturbed Krein Laplacians, let $-\Delta_{D,\Omega}$ be the Dirichlet Laplacian associated with an open set $\Omega \subset \mathbb{R}^n$, and denote by $N_{D,\Omega}(\lambda)$ the corresponding spectral distribution function (i.e., the number of eigenvalues of $-\Delta_{D,\Omega}$ not exceeding λ). The study of the asymptotic behavior of $N_{D,\Omega}(\lambda)$ as $\lambda \to \infty$ has been initiated by Weyl in 1911–1913 (cf. [189], [188], and the references in [190]), in response to a question posed in 1908 by the physicist Lorentz, pertaining to the equipartition of energy in statistical mechanics. When $n = 2$ and Ω is a bounded domain with a piecewise smooth boundary, Weyl has shown that

$$N_{D,\Omega}(\lambda) = \frac{|\Omega|}{4\pi}\lambda + o(\lambda) \text{ as } \lambda \to \infty, \tag{1.16}$$

along with the three-dimensional analogue of (1.16). (We recall our convention to denote the volume of $\Omega \subset \mathbb{R}^n$ by $|\Omega|$.) In particular, this allowed him to complete a partial proof of Rayleigh, going back to 1903. This ground-breaking work has stimulated a great deal of activity in the intervening years, in which a large number of authors have provided sharper estimates for the remainder, and considered more general elliptic operators equipped with a variety of boundary conditions.

For a general elliptic differential operator $\mathcal{A}$ of order $2m$ ($m \in \mathbb{N}$), with smooth coefficients, acting on a smooth subdomain Ω of an n-dimensional smooth manifold, spectral asymptotics of the form

$$N_{D,\Omega}(\mathcal{A};\lambda) = (2\pi)^{-n}\biggl(\int_\Omega dx \int_{a^0(x,\xi)<1} d\xi\biggr)\lambda^{n/(2m)} + O\bigl(\lambda^{(n-1)/(2m)}\bigr) \text{ as } \lambda \to \infty, \tag{1.17}$$

where $a^0(x,\xi)$ denotes the principal symbol of $\mathcal{A}$, have then been subsequently established in increasing generality (a nice exposition can be found in [6]). At the same time, it has been realized that, as the smoothness of the domain Ω (by which we mean smoothness of the boundary of Ω) and the coefficients of $\mathcal{A}$ deteriorate, the degree of detail with which the remainder can be described decreases accordingly. Indeed, the smoothness of the boundary of the underlying domain Ω affects both the nature of the remainder in (1.17), as well as the types of differential operators and boundary conditions for which such an asymptotic formula holds. Understanding this correlation then became a central theme of research. For example, in the case of the Laplacian in an arbitrary bounded, open subset Ω of $\mathbb{R}^n$, Birman and Solomyak have shown in [40] (see also [41], [42], [43], [44]) that the following Weyl asymptotic formula holds

$$N_{D,\Omega}(\lambda) = (2\pi)^{-n} v_n |\Omega|\, \lambda^{n/2} + o\bigl(\lambda^{n/2}\bigr) \text{ as } \lambda \to \infty, \tag{1.18}$$

where v_n denotes the volume of the unit ball in $\mathbb{R}^n$, and $|\Omega|$ stands for the n-dimensional Euclidean volume of Ω. (Actually, (1.18) extends to unbounded Ω with finite volume $|\Omega|$, but this will not be addressed in this survey.) On the other hand, it is known that (1.18) may fail for the Neumann Laplacian $-\Delta_{N,\Omega}$. Furthermore, if $\alpha \in (0,1)$ then Netrusov and Safarov have proved that

$$\Omega \in \mathrm{Lip}_\alpha \text{ implies } N_{D,\Omega}(\lambda) = (2\pi)^{-n} v_n |\Omega|\, \lambda^{n/2} + O\bigl(\lambda^{(n-\alpha)/2}\bigr) \text{ as } \lambda \to \infty, \tag{1.19}$$

where Lip_α is the class of bounded domains whose boundaries can be locally described by means of graphs of functions satisfying a Hölder condition of order α; this result is sharp. See [149] where this intriguing result (along with others, similar in spirit) has been obtained. Surprising connections between Weyl's asymptotic formula and geometric measure theory have been explored in [57], [109], [128] for fractal domains. Collectively, this body of work shows that the nature of the Weyl asymptotic formula is intimately related not only to the geometrical properties of the domain (as well as the type of boundary conditions), but also to the smoothness properties of its boundary (the monographs by Ivrii [112] and Safarov and Vassiliev [167] contain a wealth of information on this circle of ideas).

These considerations are by no means limited to the Laplacian; see [58] for the case of the Stokes operator, and [39], [45] for the case the Maxwell system in nonsmooth domains. However, even in the case of the Laplace operator, besides $-\Delta_{D,\Omega}$ and $-\Delta_{N,\Omega}$ there is a multitude of other concrete extensions of the Laplacian $-\Delta$ on $C_0^\infty(\Omega)$ as a nonnegative, self-adjoint operator in $L^2(\Omega; d^n x)$.

The smallest (in the operator theoretic order sense) such realization has been introduced, in an abstract setting, by M. Krein [124]. Later it was realized that in the case where the symmetric operator, whose self-adjoint extensions are sought, has a strictly positive lower bound, Krein's construction coincides with one that von Neumann had discussed in his seminal paper [183] in 1929.

For the purpose of this introduction we now briefly recall the construction of the Krein–von Neumann extension of appropriate $L^2(\Omega; d^n x)$-realizations of the differential operator $\mathcal{A}$ of order $2m$, $m \in \mathbb{N}$,

$$\mathcal{A} = \sum_{0 \le |\alpha| \le 2m} a_\alpha(\cdot) D^\alpha, \tag{1.20}$$

$$D^\alpha = (-i\partial/\partial x_1)^{\alpha_1} \cdots (-i\partial/\partial x_n)^{\alpha_n}, \quad \alpha = (\alpha_1, \dots, \alpha_n) \in \mathbb{N}_0^n, \tag{1.21}$$

$$a_\alpha(\cdot) \in C^\infty(\overline{\Omega}), \quad C^\infty(\overline{\Omega}) = \bigcap_{k \in \mathbb{N}_0} C^k(\overline{\Omega}), \tag{1.22}$$

where $\Omega \subset \mathbb{R}^n$ is a bounded C^∞ domain. Introducing the particular $L^2(\Omega; d^n x)$-realization $A_{c,\Omega}$ of $\mathcal{A}$ defined by

$$A_{c,\Omega} u = \mathcal{A} u, \quad u \in \operatorname{dom}(A_{c,\Omega}) := C_0^\infty(\Omega), \tag{1.23}$$

we assume the coefficients a_α in $\mathcal{A}$ are chosen such that $A_{c,\Omega}$ is symmetric,

$$(u, A_{c,\Omega} v)_{L^2(\Omega; d^n x)} = (A_{c,\Omega} u, v)_{L^2(\Omega; d^n x)}, \quad u, v \in C_0^\infty(\Omega), \tag{1.24}$$

has a (strictly) positive lower bound, that is, there exists $\kappa_0 > 0$ such that

$$(u, A_{c,\Omega} u)_{L^2(\Omega; d^n x)} \ge \kappa_0 \, \|u\|^2_{L^2(\Omega; d^n x)}, \quad u \in C_0^\infty(\Omega), \tag{1.25}$$

and is strongly elliptic, that is, there exists $\kappa_1 > 0$ such that

$$a^0(x,\xi) := \operatorname{Re}\Bigg(\sum_{|\alpha| = 2m} a_\alpha(x) \xi^\alpha\Bigg) \ge \kappa_1 \, |\xi|^{2m}, \quad x \in \overline{\Omega}, \ \xi \in \mathbb{R}^n. \tag{1.26}$$

Next, let $A_{\min,\Omega}$ and $A_{\max,\Omega}$ be the $L^2(\Omega; d^n x)$-realizations of $\mathcal{A}$ with domains (cf. [6], [100])

$$\operatorname{dom}(A_{\min,\Omega}) := H_0^{2m}(\Omega), \tag{1.27}$$

$$\operatorname{dom}(A_{\max,\Omega}) := \big\{ u \in L^2(\Omega; d^n x) \, \big| \, \mathcal{A} u \in L^2(\Omega; d^n x) \big\}. \tag{1.28}$$

Throughout this manuscript, $H^s(\Omega)$ denotes the L^2-based Sobolev space of order $s \in \mathbb{R}$ in Ω, and $H_0^s(\Omega)$ is the subspace of $H^s(\mathbb{R}^n)$ consisting of distributions supported in $\overline{\Omega}$ (for $s > \frac{1}{2}$, $\big(s - \frac{1}{2}\big) \notin \mathbb{N}$, the space $H_0^s(\Omega)$ can be alternatively described as the closure of $C_0^\infty(\Omega)$ in $H^s(\Omega)$). Given that the domain Ω is smooth, elliptic regularity implies

$$(A_{\min,\Omega})^* = A_{\max,\Omega} \ \text{ and } \ \overline{A_{c,\Omega}} = A_{\min,\Omega}. \tag{1.29}$$

Functional analytic considerations (cf. the discussion in Section 2) dictate that the Krein–von Neumann (sometimes also called the "soft") extension $A_{K,\Omega}$ of $A_{c,\Omega}$

on $C_0^\infty(\Omega)$ is the $L^2(\Omega;d^nx)$-realization of $A_{c,\Omega}$ with domain (cf. (2.10) derived abstractly by Krein)

$$\operatorname{dom}(A_{K,\Omega}) = \operatorname{dom}\big(\overline{A_{c,\Omega}}\big) \dotplus \ker\big((A_{c,\Omega})^*\big). \tag{1.30}$$

Above and elsewhere, $X \dotplus Y$ denotes the direct sum of two subspaces, X and Y, of a larger space Z, with the property that $X\cap Y=\{0\}$. Thus, granted (1.29), we have

$$\begin{aligned}\operatorname{dom}(A_{K,\Omega}) &= \operatorname{dom}(A_{\min,\Omega}) \dotplus \ker(A_{\max,\Omega})\\ &= H_0^{2m}(\Omega) \dotplus \big\{u\in L^2(\Omega;d^nx)\,\big|\,Au=0 \text{ in } \Omega\big\}.\end{aligned} \tag{1.31}$$

In summary, for domains with smooth boundaries, $A_{K,\Omega}$ is the self-adjoint realization of $A_{c,\Omega}$ with domain given by (1.31).

Denote by $\gamma_D^m u := \big(\gamma_N^j u\big)_{0\le j\le m-1}$ the Dirichlet trace operator of order $m\in\mathbb{N}$ (where ν denotes the outward unit normal to Ω and $\gamma_N u := \partial_\nu u$ stands for the normal derivative, or Neumann trace), and let $A_{D,\Omega}$ be the Dirichlet (sometimes also called the "hard") realization of $A_{c,\Omega}$ in $L^2(\Omega;d^nx)$ with domain

$$\operatorname{dom}(A_{D,\Omega}) := \big\{u\in H^{2m}(\Omega)\,\big|\,\gamma_D^m u=0\big\}. \tag{1.32}$$

Then $A_{K,\Omega}$, $A_{D,\Omega}$ are "extremal" in the following sense: Any nonnegative self-adjoint extension $\widetilde{A}$ in $L^2(\Omega;d^nx)$ of $A_{c,\Omega}$ (cf. (1.23)), necessarily satisfies

$$A_{K,\Omega} \le \widetilde{A} \le A_{D,\Omega} \tag{1.33}$$

in the sense of quadratic forms (cf. the discussion surrounding (2.4)).

Returning to the case where $A_{c,\Omega} = -\Delta|_{C_0^\infty(\Omega)}$, for a bounded domain Ω with a C^∞-smooth boundary, $\partial\Omega$, the corresponding Krein–von Neumann extension admits the following description

$$\begin{aligned}&-\Delta_{K,\Omega}u := -\Delta u,\\ &u\in\operatorname{dom}(-\Delta_{K,\Omega}) := \{v\in\operatorname{dom}(-\Delta_{\max,\Omega})\,|\,\gamma_N v + M_{D,N,\Omega}(\gamma_D v)=0\},\end{aligned} \tag{1.34}$$

where $M_{D,N,\Omega}$ is (up to a minus sign) an energy-dependent Dirichlet-to-Neumann map, or Weyl–Titchmarsh operator for the Laplacian. Compared with (1.31), the description (1.34) has the advantage of making explicit the boundary condition implicit in the definition of membership to $\operatorname{dom}(-\Delta_{K,\Omega})$. Nonetheless, as opposed to the classical Dirichlet and Neumann boundary condition, this turns out to be *nonlocal* in nature, as it involves $M_{D,N,\Omega}$ which, when Ω is smooth, is a boundary pseudodifferential operator of order 1. Thus, informally speaking, (1.34) is the realization of the Laplacian with the boundary condition

$$\partial_\nu u = \partial_\nu H(u) \ \text{ on } \ \partial\Omega, \tag{1.35}$$

where, given a reasonable function w in Ω, $H(w)$ is the harmonic extension of the Dirichlet boundary trace $\gamma_D^0 w$ to Ω (cf. (4.15)).

While at first sight the nonlocal boundary condition $\gamma_N v + M_{D,N,\Omega}(\gamma_D v)=0$ in (1.34) for the Krein Laplacian $-\Delta_{K,\Omega}$ may seem familiar from the abstract approach to self-adjoint extensions of semibounded symmetric operators within the theory of boundary value spaces, there are some crucial distinctions in the concrete case of Laplacians on (nonsmooth) domains which will be delineated at the end of Section 6.

For rough domains, matters are more delicate as the nature of the boundary trace operators and the standard elliptic regularity theory are both fundamentally affected. Following work in [89], here we shall consider the class of *quasi-convex domains*. The latter is the subclass of bounded, Lipschitz domains in $\mathbb{R}^n$ characterized by the demand that

(i) there exists a sequence of relatively compact, C^2-subdomains exhausting the original domain, and whose second fundamental forms are bounded from below in a uniform fashion (for a precise formulation see Definition 5.3),

or

(ii) near every boundary point there exists a suitably small $\delta > 0$, such that the boundary is given by the graph of a function $\varphi : \mathbb{R}^{n-1} \to \mathbb{R}$ (suitably rotated and translated) which is Lipschitz and whose derivative satisfy the pointwise $H^{1/2}$-multiplier condition

$$\begin{aligned} &\sum_{k=1}^{n-1} \|f_k\, \partial_k \varphi_j\|_{H^{1/2}(\mathbb{R}^{n-1})} \\ &\quad \leq \delta \sum_{k=1}^{n-1} \|f_k\|_{H^{1/2}(\mathbb{R}^{n-1})}, \quad f_1, \dots, f_{n-1} \in H^{1/2}(\mathbb{R}^{n-1}). \end{aligned} \tag{1.36}$$

See Hypothesis 5.7 for a precise formulation. In particular, (1.36) is automatically satisfied when $\omega(\nabla\varphi, t)$, the modulus of continuity of $\nabla\varphi$ at scale t, satisfies the square-Dini condition (compare to [140], [141], where this type of domain was introduced and studied),

$$\int_0^1 \Big(\frac{\omega(\nabla\varphi; t)}{t^{1/2}}\Big)^2 \frac{dt}{t} < \infty. \tag{1.37}$$

In turn, (1.37) is automatically satisfied if the Lipschitz function φ is of class $C^{1,r}$ for some $r > 1/2$. As a result, examples of quasi-convex domains include:

(i) All bounded (geometrically) convex domains.
(ii) All bounded Lipschitz domains satisfying a uniform exterior ball condition (which, informally speaking, means that a ball of fixed radius can be "rolled" along the boundary).
(iii) All open sets which are the image of a domain as in $(i), (ii)$ above under a $C^{1,1}$-diffeomorphism.
(iv) All bounded domains of class $C^{1,r}$ for some $r > 1/2$.

We note that being quasi-convex is a local property of the boundary. The philosophy behind this concept is that Lipschitz-type singularities are allowed in the boundary as long as they are directed outwardly (see Figure 1 on p. 43). The key feature of this class of domains is the fact that the classical elliptic regularity property

$$\mathrm{dom}(-\Delta_{D,\Omega}) \subset H^2(\Omega), \quad \mathrm{dom}(-\Delta_{N,\Omega}) \subset H^2(\Omega) \tag{1.38}$$

remains valid. In this vein, it is worth recalling that the presence of a single re-entrant corner for the domain Ω invalidates (1.38). All our results in this survey are actually valid for the class of bounded Lipschitz domains for which (1.38) holds. Condition (1.38) is, however, a regularity assumption on the boundary of the Lipschitz domain Ω and the class of quasi-convex domains is the largest one for which we know (1.38) to hold. Under the hypothesis of quasi-convexity, it has been shown in [89] that the Krein Laplacian $-\Delta_{K,\Omega}$ (i.e., the Krein–von Neumann extension of the Laplacian $-\Delta$ defined on $C_0^\infty(\Omega)$) in (1.34) is a well-defined self-adjoint operator which agrees with the operator constructed using the recipe in (1.31).

The main issue of this survey is the study of the spectral properties of $H_{K,\Omega}$, the Krein–von Neumann extension of the perturbed Laplacian

$$-\Delta + V \ \text{ on } \ C_0^\infty(\Omega), \tag{1.39}$$

in the case where both the potential V and the domain Ω are nonsmooth. As regards the former, we shall assume that $0 \leq V \in L^\infty(\Omega; d^n x)$, and we shall assume that $\Omega \subset \mathbb{R}^n$ is a quasi-convex domain (more on this shortly). In particular, we wish to clarify the extent to which a Weyl asymptotic formula continues to hold for this operator. For us, this undertaking was originally inspired by the discussion by Alonso and Simon in [14]. At the end of that paper, the authors comment to the effect that *"It seems to us that the Krein extension of $-\Delta$, i.e., $-\Delta$ with the boundary condition* (1.35)*, is a natural object and therefore worthy of further study. For example: Are the asymptotics of its nonzero eigenvalues given by Weyl's formula?"* Subsequently we have learned that when Ω is C^∞-smooth this has been shown to be the case by Grubb in [97]. More specifically, in that paper Grubb has proved that if $N_{K,\Omega}(\mathcal{A};\lambda)$ denotes the number of nonzero eigenvalues of $A_{K,\Omega}$ (defined as in (1.31)) not exceeding λ, then

$$\Omega \in C^\infty \ \text{ implies } \ N_{K,\Omega}(\mathcal{A};\lambda) = C_{A,n}\lambda^{n/(2m)} + O\big(\lambda^{(n-\theta)/(2m)}\big) \ \text{ as } \lambda \to \infty, \tag{1.40}$$

where, with $a^0(x,\xi)$ as in (1.26),

$$C_{A,n} := (2\pi)^{-n} \int_\Omega d^n x \int_{a^0(x,\xi)<1} d^n\xi \tag{1.41}$$

and

$$\theta := \max\left\{\frac{1}{2} - \varepsilon\,,\, \frac{2m}{2m+n-1}\right\}, \ \text{ with } \varepsilon > 0 \text{ arbitrary.} \tag{1.42}$$

See also [143], [144], and most recently, [102], where the authors derive a sharpening of the remainder in (1.40) to any $\theta < 1$. To show (1.40)–(1.42), Grubb has reduced the eigenvalue problem

$$\mathcal{A}u = \lambda\, u, \quad u \in \mathrm{dom}(A_{K,\Omega}),\ \lambda > 0, \tag{1.43}$$

to the higher-order, elliptic system

$$\begin{cases} \mathcal{A}^2 v = \lambda\, \mathcal{A} v \ \text{ in } \ \Omega, \\ \gamma_D^{2m} v = 0 \ \text{ on } \ \partial\Omega, \\ v \in C^\infty(\overline{\Omega}). \end{cases} \tag{1.44}$$

Then the strategy is to use known asymptotics for the spectral distribution function of regular elliptic boundary problems, along with perturbation results due to Birman, Solomyak, and Grubb (see the literature cited in [97] for precise references). It should be noted that the fact that the boundary of Ω and the coefficients of $\mathcal{A}$ are smooth plays an important role in Grubb's proof. First, this is used to ensure that (1.29) holds which, in turn, allows for the concrete representation (1.31) (a formula which in effect lies at the start of the entire theory, as Grubb adopts this as the *definition* of the domains of the Krein–von Neumann extension). In addition, at a more technical level, Lemma 3 in [97] is justified by making appeal to the theory of pseudo-differential operators on $\partial\Omega$, assumed to be an $(n-1)$-dimensional C^∞ manifold. In our case, that is, when dealing with the Krein–von Neumann extension of the perturbed Laplacian (1.39), we establish the following theorem:

Theorem 1.1. *Let $\Omega \subset \mathbb{R}^n$ be a quasi-convex domain, assume that $0 \leq V \in L^\infty(\Omega; d^n x)$, and denote by $H_{K,\Omega}$ the Krein–von Neumann extension of the perturbed Laplacian* (1.39)*. Then there exists a sequence of numbers*

$$0 < \lambda_{K,\Omega,1} \leq \lambda_{K,\Omega,2} \leq \cdots \leq \lambda_{K,\Omega,j} \leq \lambda_{K,\Omega,j+1} \leq \cdots \tag{1.45}$$

converging to infinity, with the following properties.

(i) *The spectrum of $H_{K,\Omega}$ is given by*

$$\sigma(H_{K,\Omega}) = \{0\} \cup \{\lambda_{K,\Omega,j}\}_{j\in\mathbb{N}}, \tag{1.46}$$

and each number $\lambda_{K,\Omega,j}$, $j \in \mathbb{N}$, is an eigenvalue for $H_{K,\Omega}$ of finite multiplicity.

(ii) *There exists a countable family of orthonormal eigenfunctions for $H_{K,\Omega}$ which span the orthogonal complement of the kernel of this operator. More precisely, there exists a collection of functions $\{w_j\}_{j\in\mathbb{N}}$ with the following properties:*

$$w_j \in \operatorname{dom}(H_{K,\Omega}) \ \text{ and } \ H_{K,\Omega} w_j = \lambda_{K,\Omega,j} w_j, \ j \in \mathbb{N}, \tag{1.47}$$

$$(w_j, w_k)_{L^2(\Omega;d^n x)} = \delta_{j,k}, \ j,k \in \mathbb{N}, \tag{1.48}$$

$$L^2(\Omega; d^n x) = \ker(H_{K,\Omega}) \oplus \overline{\text{lin. span}\{w_j\}_{j\in\mathbb{N}}}, \quad (\textit{orthogonal direct sum}). \tag{1.49}$$

If V is Lipschitz then $w_j \in H^{1/2}(\Omega)$ for every j and, in fact, $w_j \in C^\infty(\overline{\Omega})$ for every j if Ω is C^∞ and $V \in C^\infty(\overline{\Omega})$.

(iii) *The following min-max principle holds:*

$$\lambda_{K,\Omega,j} = \min_{\substack{W_j \text{ subspace of } H_0^2(\Omega) \\ \dim(W_j)=j}} \left(\max_{0\neq u\in W_j} \left(\frac{\|(-\Delta+V)u\|^2_{L^2(\Omega;d^nx)}}{\|\nabla u\|^2_{(L^2(\Omega;d^nx))^n} + \|V^{1/2}u\|^2_{L^2(\Omega;d^nx)}} \right)\right), \quad j\in\mathbb{N}. \tag{1.50}$$

(iv) *If*

$$0 < \lambda_{D,\Omega,1} \leq \lambda_{D,\Omega,2} \leq \cdots \leq \lambda_{D,\Omega,j} \leq \lambda_{D,\Omega,j+1} \leq \cdots \tag{1.51}$$

are the eigenvalues of the perturbed Dirichlet Laplacian $-\Delta_{D,\Omega}$ *(i.e., the Friedrichs extension of* (1.39) *in* $L^2(\Omega; d^nx)$*), listed according to their multiplicities, then*

$$0 < \lambda_{D,\Omega,j} \leq \lambda_{K,\Omega,j}, \quad j\in\mathbb{N}, \tag{1.52}$$

Consequently introducing the spectral distribution functions

$$N_{X,\Omega}(\lambda) := \#\{j\in\mathbb{N} \,|\, \lambda_{X,\Omega,j} \leq \lambda\}, \quad X\in\{D,K\}, \tag{1.53}$$

one has

$$N_{K,\Omega}(\lambda) \leq N_{D,\Omega}(\lambda). \tag{1.54}$$

(v) *Corresponding to the case* $V\equiv 0$*, the first nonzero eigenvalue* $\lambda^{(0)}_{K,\Omega,1}$ *of* $-\Delta_{K,\Omega}$ *satisfies*

$$\lambda^{(0)}_{D,\Omega,2} \leq \lambda^{(0)}_{K,\Omega,1} \ \text{ and } \ \lambda^{(0)}_{K,\Omega,2} \leq \frac{n^2+8n+20}{(n+2)^2}\lambda^{(0)}_{K,\Omega,1}. \tag{1.55}$$

In addition,

$$\sum_{j=1}^{n} \lambda^{(0)}_{K,\Omega,j+1} < (n+4)\lambda^{(0)}_{K,\Omega,1} - \frac{4}{n+4}(\lambda^{(0)}_{K,\Omega,2} - \lambda^{(0)}_{K,\Omega,1}) \leqslant (n+4)\lambda^{(0)}_{K,\Omega,1}, \tag{1.56}$$

and

$$\sum_{j=1}^{k} \big(\lambda^{(0)}_{K,\Omega,k+1} - \lambda^{(0)}_{K,\Omega,j}\big)^2 \leq \frac{4(n+2)}{n^2} \sum_{j=1}^{k} \big(\lambda^{(0)}_{K,\Omega,k+1} - \lambda^{(0)}_{K,\Omega,j}\big)\lambda^{(0)}_{K,\Omega,j} \quad k\in\mathbb{N}. \tag{1.57}$$

Moreover, if Ω *is a bounded, convex domain in* $\mathbb{R}^n$*, then the first two Dirichlet eigenvalues and the first nonzero eigenvalue of the Krein Laplacian in* Ω *satisfy*

$$\lambda^{(0)}_{D,\Omega,2} \leq \lambda^{(0)}_{K,\Omega,1} \leq 4\,\lambda^{(0)}_{D,\Omega,1}. \tag{1.58}$$

(vi) *The following Weyl asymptotic formula holds:*

$$N_{K,\Omega}(\lambda) = (2\pi)^{-n} v_n |\Omega|\, \lambda^{n/2} + O\big(\lambda^{(n-(1/2))/2}\big) \ \text{ as } \ \lambda\to\infty, \tag{1.59}$$

where, as before, v_n *denotes the volume of the unit ball in* $\mathbb{R}^n$*, and* $|\Omega|$ *stands for the* n*-dimensional Euclidean volume of* Ω*.*

This theorem answers the question posed by Alonso and Simon in [14] (which corresponds to $V \equiv 0$), and further extends the work by Grubb in [97] in the sense that we allow nonsmooth domains and coefficients. To prove this result, we adopt Grubb's strategy and show that the eigenvalue problem

$$(-\Delta + V)u = \lambda\, u, \quad u \in \mathrm{dom}(H_{K,\Omega}),\ \lambda > 0, \tag{1.60}$$

is equivalent to the following fourth-order problem

$$\begin{cases} (-\Delta + V)^2 w = \lambda\,(-\Delta + V)w \ \text{ in } \ \Omega, \\ \ \gamma_D w = \gamma_N w = 0 \ \text{ on } \ \partial\Omega, \\ w \in \mathrm{dom}(-\Delta_{\max}). \end{cases} \tag{1.61}$$

This is closely related to the so-called problem of the *buckling of a clamped plate*,

$$\begin{cases} -\Delta^2 w = \lambda\,\Delta w \ \text{ in } \ \Omega, \\ \gamma_D w = \gamma_N w = 0 \ \text{ on } \ \partial\Omega, \\ w \in \mathrm{dom}(-\Delta_{\max}), \end{cases} \tag{1.62}$$

to which (1.61) reduces when $V \equiv 0$. From a physical point of view, the nature of the later boundary value problem can be described as follows. In the two-dimensional setting, the bifurcation problem for a clamped, homogeneous plate in the shape of Ω, with uniform lateral compression on its edges has the eigenvalues λ of the problem (1.61) as its critical points. In particular, the first eigenvalue of (1.61) is proportional to the load compression at which the plate buckles.

One of the upshots of our work in this context is establishing a definite connection between the Krein–von Neumann extension of the Laplacian and the buckling problem (1.62). In contrast to the smooth case, since in our setting the solution w of (1.61) does not exhibit any extra regularity on the Sobolev scale $H^s(\Omega)$, $s \geq 0$, other than membership to $L^2(\Omega; d^n x)$, a suitable interpretation of the boundary conditions in (1.61) should be adopted. (Here we shall rely on the recent progress from [89] where this issue has been resolved by introducing certain novel boundary Sobolev spaces, well adapted to the class of Lipschitz domains.) We nonetheless find this trade-off, between the 2nd-order boundary problem (1.60) which has nonlocal boundary conditions, and the boundary problem (1.61) which has local boundary conditions, but is of fourth-order, very useful. The reason is that (1.61) can be rephrased, in view of (1.38) and related regularity results developed in [89], in the form of

$$(-\Delta + V)^2 u = \lambda\,(-\Delta + V)u \ \text{ in } \ \Omega, \quad u \in H^2_0(\Omega). \tag{1.63}$$

In principle, this opens the door to bringing onto the stage the theory of generalized eigenvalue problems, that is, operator pencil problems of the form

$$Tu = \lambda\, Su, \tag{1.64}$$

where T and S are certain linear operators in a Hilbert space. Abstract results of this nature can be found for instance, in [133], [156], [175] (see also [129], [130], where this is applied to the asymptotic distribution of eigenvalues). We, however, find it more convenient to appeal to a version of (1.64) which emphasizes the role of the symmetric forms

$$a(u,v) := \int_\Omega d^n x\, \overline{(-\Delta + V)u}\,(-\Delta + V)v, \quad u,v \in H_0^2(\Omega), \tag{1.65}$$

$$b(u,v) := \int_\Omega d^n x\, \overline{\nabla u} \cdot \nabla v + \int_\Omega d^n x\, \overline{V^{1/2} u}\, V^{1/2} v, \quad u,v \in H_0^2(\Omega), \tag{1.66}$$

and reformulate (1.63) as the problem of finding $u \in H_0^2(\Omega)$ which satisfies

$$a(u,v) = \lambda\, b(u,v) \quad v \in H_0^2(\Omega). \tag{1.67}$$

This type of eigenvalue problem, in the language of bilinear forms associated with differential operators, has been studied by Kozlov in a series of papers [118], [119], [120]. In particular, in [120], Kozlov has obtained Weyl asymptotic formulas in the case where the underlying domain Ω in (1.65) is merely Lipschitz, and the lower-order coefficients of the quadratic forms (1.65)–(1.66) are only measurable and bounded (see Theorem 9.1 for a precise formulation). Our demand that the potential V is in $L^\infty(\Omega; d^n x)$ is therefore inherited from Kozlov's theorem. Based on this result and the fact that the problems (1.65)–(1.67) and (1.60) are spectral-equivalent, we can then conclude that (1.59) holds. Formulas (1.55)–(1.57) are also a byproduct of the connection between (1.60) and (1.61) and known spectral estimates for the buckling plate problem from [27], [28], [31], [60], [110], [150], [152], [153]. Similarly, (1.58) for convex domains is based on the connection between (1.60) and (1.61) and the eigenvalue inequality relating the first eigenvalue of a fixed membrane and that of the buckling problem for the clamped plate as proven in [151] (see also [152], [153]).

In closing, we wish to point out that in the C^∞-smooth setting, Grubb's remainder in (1.40), with the improvement to any $\theta < 1$ in [102], [143], [144], is sharper than that in (1.59). However, the main novel feature of our Theorem 1.1 is the low regularity assumptions on the underlying domain Ω, and the fact that we allow a nonsmooth potential V. As was the case with the Weyl asymptotic formula for the classical Dirichlet and Neumann Laplacians (briefly reviewed at the beginning of this section), the issue of regularity (or lack thereof) has always been of considerable importance in this line of work (as early as 1970, Birman and Solomyak noted in [40] that "*there has been recently some interest in obtaining the classical asymptotic spectral formulas under the weakest possible hypotheses.*"). The interested reader may consult the paper [44] by Birman and Solomyak (see also [42], [43]), as well as the article [63] by Davies for some very readable, highly informative surveys underscoring this point (collectively, these papers also contain more than 500 references concerning this circle of ideas).

We note that the results in Sections 4–6 originally appeared in [89], while those in Sections 7–11 originally appeared in [29].

Finally, a notational comment: For obvious reasons in connection with quantum mechanical applications, we will, with a slight abuse of notation, dub $-\Delta$ (rather than Δ) as the "Laplacian" in this survey.

2. The abstract Krein–von Neumann extension

To get started, we briefly elaborate on the notational conventions used throughout this survey and especially throughout this section which collects abstract material on the Krein–von Neumann extension. Let $\mathcal{H}$ be a separable complex Hilbert space, $(\,\cdot\,,\,\cdot\,)_{\mathcal{H}}$ the scalar product in $\mathcal{H}$ (linear in the second factor), and $I_{\mathcal{H}}$ the identity operator in $\mathcal{H}$. Next, let T be a linear operator mapping (a subspace of) a Banach space into another, with $\operatorname{dom}(T)$ and $\operatorname{ran}(T)$ denoting the domain and range of T. The closure of a closable operator S is denoted by $\overline{S}$. The kernel (null space) of T is denoted by $\ker(T)$. The spectrum, essential spectrum, and resolvent set of a closed linear operator in $\mathcal{H}$ will be denoted by $\sigma(\cdot)$, $\sigma_{\rm ess}(\cdot)$, and $\rho(\cdot)$, respectively. The Banach spaces of bounded and compact linear operators on $\mathcal{H}$ are denoted by $\mathcal{B}(\mathcal{H})$ and $\mathcal{B}_\infty(\mathcal{H})$, respectively. Similarly, the Schatten–von Neumann (trace) ideals will subsequently be denoted by $\mathcal{B}_p(\mathcal{H})$, $p \in (0,\infty)$. The analogous notation $\mathcal{B}(\mathcal{X}_1,\mathcal{X}_2)$, $\mathcal{B}_\infty(\mathcal{X}_1,\mathcal{X}_2)$, etc., will be used for bounded, compact, etc., operators between two Banach spaces $\mathcal{X}_1$ and $\mathcal{X}_2$. Moreover, $\mathcal{X}_1 \hookrightarrow \mathcal{X}_2$ denotes the continuous embedding of the Banach space $\mathcal{X}_1$ into the Banach space $\mathcal{X}_2$. In addition, $U_1 \dotplus U_2$ denotes the direct sum of the subspaces U_1 and U_2 of a Banach space $\mathcal{X}$; and $V_1 \oplus V_2$ represents the orthogonal direct sum of the subspaces V_j, $j = 1, 2$, of a Hilbert space $\mathcal{H}$.

Throughout this manuscript, if X denotes a Banach space, X^* denotes the *adjoint space* of continuous conjugate linear functionals on X, that is, the *conjugate dual space* of X (rather than the usual dual space of continuous linear functionals on X). This avoids the well-known awkward distinction between adjoint operators in Banach and Hilbert spaces (cf., e.g., the pertinent discussion in [71, p. 3, 4]).

Given a reflexive Banach space $\mathcal{V}$ and $T \in \mathcal{B}(\mathcal{V},\mathcal{V}^*)$, the fact that T is self-adjoint is defined by the requirement that

$$ {}_{\mathcal{V}}\langle u, Tv\rangle_{\mathcal{V}^*} = {}_{\mathcal{V}^*}\langle Tu, v\rangle_{\mathcal{V}} = \overline{{}_{\mathcal{V}}\langle v, Tu\rangle_{\mathcal{V}^*}}, \quad u, v \in \mathcal{V}, \tag{2.1}$$

where in this context bar denotes complex conjugation, $\mathcal{V}^*$ is the conjugate dual of $\mathcal{V}$, and ${}_{\mathcal{V}}\langle\,\cdot\,,\,\cdot\,\rangle_{\mathcal{V}^*}$ stands for the $\mathcal{V},\mathcal{V}^*$ pairing.

A linear operator $S : \operatorname{dom}(S) \subseteq \mathcal{H} \to \mathcal{H}$, is called *symmetric*, if

$$ (u, Sv)_{\mathcal{H}} = (Su, v)_{\mathcal{H}}, \quad u, v \in \operatorname{dom}(S). \tag{2.2}$$

If $\operatorname{dom}(S) = \mathcal{H}$, the classical Hellinger–Toeplitz theorem guarantees that $S \in \mathcal{B}(\mathcal{H})$, in which situation S is readily seen to be self-adjoint. In general, however, symmetry is a considerably weaker property than self-adjointness and a classical problem in functional analysis is that of determining all self-adjoint extensions in $\mathcal{H}$ of a given unbounded symmetric operator of equal and nonzero deficiency indices. (Here self-adjointness of an operator $\widetilde{S}$ in $\mathcal{H}$, is of course defined as usual by $\big(\widetilde{S}\big)^* = \widetilde{S}$.) In this manuscript we will be particularly interested in this question within the class of densely defined (i.e., $\overline{\operatorname{dom}(S)} = \mathcal{H}$), nonnegative operators (in fact, in most instances S will even turn out to be strictly positive) and we focus almost exclusively on self-adjoint extensions that are nonnegative operators. In the latter scenario, there are two distinguished constructions which we will briefly review next.

To set the stage, we recall that a linear operator $S : \mathrm{dom}(S) \subseteq \mathcal{H} \to \mathcal{H}$ is called *nonnegative* provided

$$(u, Su)_{\mathcal{H}} \geq 0, \quad u \in \mathrm{dom}(S). \tag{2.3}$$

(In particular, S is symmetric in this case.) S is called *strictly positive*, if for some $\varepsilon > 0$, $(u, Su)_{\mathcal{H}} \geq \varepsilon \|u\|_{\mathcal{H}}^2$, $u \in \mathrm{dom}(S)$. Next, we recall that $A \leq B$ for two self-adjoint operators in $\mathcal{H}$ if

$$\begin{aligned} &\mathrm{dom}\big(|A|^{1/2}\big) \supseteq \mathrm{dom}\big(|B|^{1/2}\big) \text{ and} \\ &\big(|A|^{1/2}u, U_A|A|^{1/2}u\big)_{\mathcal{H}} \leq \big(|B|^{1/2}u, U_B|B|^{1/2}u\big)_{\mathcal{H}}, \quad u \in \mathrm{dom}\big(|B|^{1/2}\big), \end{aligned} \tag{2.4}$$

where U_C denotes the partial isometry in $\mathcal{H}$ in the polar decomposition of a densely defined closed operator C in $\mathcal{H}$, $C = U_C|C|$, $|C| = (C^*C)^{1/2}$. (If in addition, C is self-adjoint, then U_C and $|C|$ commute.) We also recall ([75, Section I.6], [114, Theorem VI.2.21]) that if A and B are both self-adjoint and nonnegative in $\mathcal{H}$, then

$$0 \leq A \leq B \text{ if and only if } (B + aI_{\mathcal{H}})^{-1} \leq (A + aI_{\mathcal{H}})^{-1} \text{ for all } a > 0, \tag{2.5}$$

(which implies $0 \leq A^{1/2} \leq B^{1/2}$) and

$$\ker(A) = \ker\big(A^{1/2}\big) \tag{2.6}$$

(with $C^{1/2}$ the unique nonnegative square root of a nonnegative self-adjoint operator C in $\mathcal{H}$).

For simplicity we will always adhere to the conventions that S is a linear, unbounded, densely defined, nonnegative (i.e., $S \geq 0$) operator in $\mathcal{H}$, and that S has nonzero deficiency indices. In particular,

$$\mathrm{def}(S) = \dim(\ker(S^* - zI_{\mathcal{H}})) \in \mathbb{N} \cup \{\infty\}, \quad z \in \mathbb{C}\backslash[0, \infty), \tag{2.7}$$

is well known to be independent of z. Moreover, since S and its closure $\overline{S}$ have the same self-adjoint extensions in $\mathcal{H}$, we will without loss of generality assume that S is closed in the remainder of this section.

The following is a fundamental result to be found in M. Krein's celebrated 1947 paper [124] (cf. also Theorems 2 and 5–7 in the English summary on page 492):

Theorem 2.1. *Assume that S is a densely defined, closed, nonnegative operator in $\mathcal{H}$. Then, among all nonnegative self-adjoint extensions of S, there exist two distinguished ones, S_K and S_F, which are, respectively, the smallest and largest* (*in the sense of order between self-adjoint operators, cf.* (2.4)) *such extension. Furthermore, a nonnegative self-adjoint operator $\widetilde{S}$ is a self-adjoint extension of S if and only if $\widetilde{S}$ satisfies*

$$S_K \leq \widetilde{S} \leq S_F. \tag{2.8}$$

In particular, (2.8) *determines S_K and S_F uniquely.*

In addition, if $S \geq \varepsilon I_{\mathcal{H}}$ *for some* $\varepsilon > 0$*, one has* $S_F \geq \varepsilon I_{\mathcal{H}}$*, and*

$$\operatorname{dom}(S_F) = \operatorname{dom}(S) \dotplus (S_F)^{-1} \ker(S^*), \tag{2.9}$$

$$\operatorname{dom}(S_K) = \operatorname{dom}(S) \dotplus \ker(S^*), \tag{2.10}$$

$$\begin{aligned}\operatorname{dom}(S^*) &= \operatorname{dom}(S) \dotplus (S_F)^{-1} \ker(S^*) \dotplus \ker(S^*) \\ &= \operatorname{dom}(S_F) \dotplus \ker(S^*),\end{aligned} \tag{2.11}$$

in particular,

$$\ker(S_K) = \ker\big((S_K)^{1/2}\big) = \ker(S^*) = \operatorname{ran}(S)^{\perp}. \tag{2.12}$$

Here the operator inequalities in (2.8) are understood in the sense of (2.4) and hence they can equivalently be written as

$$(S_F + aI_{\mathcal{H}})^{-1} \leqslant \big(\widetilde{S} + aI_{\mathcal{H}}\big)^{-1} \leqslant (S_K + aI_{\mathcal{H}})^{-1} \text{ for some (and hence for all) } a > 0. \tag{2.13}$$

We will call the operator S_K the *Krein–von Neumann extension* of S. See [124] and also the discussion in [14], [23], [24]. It should be noted that the Krein–von Neumann extension was first considered by von Neumann [183] in 1929 in the case where S is strictly positive, that is, if $S \geq \varepsilon I_{\mathcal{H}}$ for some $\varepsilon > 0$. (His construction appears in the proof of Theorem 42 on pages 102–103.) However, von Neumann did not isolate the extremal property of this extension as described in (2.8) and (2.13). M. Krein [124], [125] was the first to systematically treat the general case $S \geq 0$ and to study all nonnegative self-adjoint extensions of S, illustrating the special role of the *Friedrichs extension* (i.e., the "hard" extension) S_F of S and the Krein–von Neumann (i.e., the "soft") extension S_K of S as extremal cases when considering all nonnegative extensions of S. For a recent exhaustive treatment of self-adjoint extensions of semibounded operators we refer to [22]–[25].

For classical references on the subject of self-adjoint extensions of semibounded operators (not necessarily restricted to the Krein–von Neumann extension) we refer to Birman [37], [38], Friedrichs [79], Freudenthal [78], Grubb [94], [95], Krein [125], Štraus [173], and Višik [182] (see also the monographs by Akhiezer and Glazman [10, Sect. 109], Faris [75, Part III], and the recent book by Grubb [100, Sect. 13.2]).

An intrinsic description of the Friedrichs extension S_F of $S \geq 0$ due to Freudenthal [78] in 1936 describes S_F as the operator $S_F : \operatorname{dom}(S_F) \subset \mathcal{H} \to \mathcal{H}$ given by

$$\begin{aligned}&S_F u := S^* u, \\ &u \in \operatorname{dom}(S_F) := \big\{v \in \operatorname{dom}(S^*) \,\big|\, \text{there exists } \{v_j\}_{j\in\mathbb{N}} \subset \operatorname{dom}(S), \\ &\quad \text{with } \lim_{j\to\infty} \|v_j - v\|_{\mathcal{H}} = 0 \text{ and } ((v_j - v_k), S(v_j - v_k))_{\mathcal{H}} \to 0 \text{ as } j,k \to \infty\big\}.\end{aligned} \tag{2.14}$$

Then, as is well known,

$$S_F \geq 0, \tag{2.15}$$

$$\begin{aligned} &\operatorname{dom}\big((S_F)^{1/2}\big) = \big\{v \in \mathcal{H} \,\big|\, \text{there exists} \{v_j\}_{j\in\mathbb{N}} \subset \operatorname{dom}(S), \\ &\quad \text{with} \lim_{j\to\infty} \|v_j - v\|_{\mathcal{H}} = 0 \text{ and } ((v_j - v_k), S(v_j - v_k))_{\mathcal{H}} \to 0 \text{ as } j,k \to \infty\big\}, \end{aligned} \tag{2.16}$$

and

$$S_F = S^*|_{\operatorname{dom}(S^*)\cap\operatorname{dom}((S_F)^{1/2})}. \tag{2.17}$$

Equations (2.16) and (2.17) are intimately related to the definition of S_F via (the closure of) the sesquilinear form generated by S as follows: One introduces the sesquilinear form

$$q_S(f,g) = (f, Sg)_{\mathcal{H}}, \quad f,g \in \operatorname{dom}(q_S) = \operatorname{dom}(S). \tag{2.18}$$

Since $S \geq 0$, the form q_S is closable and we denote by Q_S the closure of q_S. Then $Q_S \geq 0$ is densely defined and closed. By the first and second representation theorem for forms (cf., e.g., [114, Sect. 6.2]), Q_S is uniquely associated with a nonnegative, self-adjoint operator in $\mathcal{H}$. This operator is precisely the Friedrichs extension, $S_F \geq 0$, of S, and hence,

$$\begin{aligned} &Q_S(f,g) = (f, S_F g)_{\mathcal{H}}, \quad f \in \operatorname{dom}(Q_S),\, g \in \operatorname{dom}(S_F), \\ &\operatorname{dom}(Q_S) = \operatorname{dom}\big((S_F)^{1/2}\big). \end{aligned} \tag{2.19}$$

An intrinsic description of the Krein–von Neumann extension S_K of $S \geq 0$ has been given by Ando and Nishio [16] in 1970, where S_K has been characterized as the operator $S_K : \operatorname{dom}(S_K) \subset \mathcal{H} \to \mathcal{H}$ given by

$$\begin{aligned} &S_K u := S^* u, \\ &u \in \operatorname{dom}(S_K) := \big\{v \in \operatorname{dom}(S^*) \,\big|\, \text{there exists} \{v_j\}_{j\in\mathbb{N}} \subset \operatorname{dom}(S), \\ &\quad \text{with} \lim_{j\to\infty} \|Sv_j - S^*v\|_{\mathcal{H}} = 0 \text{ and } ((v_j - v_k), S(v_j - v_k))_{\mathcal{H}} \to 0 \text{ as } j,k \to \infty\big\}. \end{aligned} \tag{2.20}$$

By (2.14) one observes that shifting S by a constant commutes with the operation of taking the Friedrichs extension of S, that is, for any $c \in \mathbb{R}$,

$$(S + cI_{\mathcal{H}})_F = S_F + cI_{\mathcal{H}}, \tag{2.21}$$

but by (2.20), the analog of (2.21) for the Krein–von Neumann extension S_K fails.

At this point we recall a result due to Makarov and Tsekanovskii [134], concerning symmetries (e.g., the rotational symmetry exploited in Section 11), and more generally, a scale invariance, shared by S, S^*, S_F, and S_K (see also [105]). Actually, we will prove a slight extension of the principal result in [134]:

Proposition 2.2. *Let $\mu > 0$, suppose that $V, V^{-1} \in \mathcal{B}(\mathcal{H})$, and assume S to be a densely defined, closed, nonnegative operator in $\mathcal{H}$ satisfying*

$$VSV^{-1} = \mu S, \tag{2.22}$$

and

$$VSV^{-1} = (V^*)^{-1}SV^* \ \ (\textit{or equivalently, } (V^*V)^{-1}S(V^*V) = S\,). \tag{2.23}$$

Then also S^*, S_F, and S_K satisfy

$$(V^*V)^{-1}S^*(V^*V) = S^*, \quad VS^*V^{-1} = \mu S^*, \tag{2.24}$$

$$(V^*V)^{-1}S_F(V^*V) = S_F, \quad VS_FV^{-1} = \mu S_F, \tag{2.25}$$

$$(V^*V)^{-1}S_K(V^*V) = S_K, \quad VS_KV^{-1} = \mu S_K. \tag{2.26}$$

Proof. Applying [185, p. 73, 74], (2.22) yields $VSV^{-1} = (V^*)^{-1}SV^*$. The latter relation is equivalent to $(V^*V)^{-1}S(V^*V) = S$ and hence also equivalent to $(V^*V)S(V^*V)^{-1} = S$. Taking adjoints (and applying [185, p. 73, 74] again) then yields $(V^*)^{-1}S^*V^* = VS^*V^{-1}$; the latter is equivalent to $(V^*V)^{-1}S^*(V^*V) = S^*$ and hence also equivalent to $(V^*V)S^*(V^*V)^{-1} = S$. Replacing S and S^* by $(V^*V)^{-1}S(V^*V)$ and $(V^*V)^{-1}S^*(V^*V)$, respectively, in (2.14), and subsequently, in (2.20), then yields that

$$(V^*V)^{-1}S_F(V^*V) = S_F \text{ and } (V^*V)^{-1}S_K(V^*V) = S_K. \tag{2.27}$$

The latter are of course equivalent to

$$(V^*V)S_F(V^*V)^{-1} = S_F \text{ and } (V^*V)S_K(V^*V)^{-1} = S_K. \tag{2.28}$$

Finally, replacing S by VSV^{-1} and S^* by VS^*V^{-1} in (2.14) then proves $VS_FV^{-1} = \mu S_F$. Performing the same replacement in (2.20) yields $VS_KV^{-1} = \mu S_K$. □

If in addition, V is unitary (implying $V^*V = I_{\mathcal{H}}$), Proposition 2.2 immediately reduces to [134, Theorem 2.2]. In this special case one can also provide a quick alternative proof by directly invoking the inequalities (2.13) and the fact that they are preserved under unitary equivalence.

Similarly to Proposition 2.2, the following results also immediately follow from the characterizations (2.14) and (2.20) of S_F and S_K, respectively:

Proposition 2.3. *Let $U\colon \mathcal{H}_1 \to \mathcal{H}_2$ be unitary from $\mathcal{H}_1$ onto $\mathcal{H}_2$ and assume S to be a densely defined, closed, nonnegative operator in $\mathcal{H}_1$ with adjoint S^*, Friedrichs extension S_F, and Krein–von Neumann extension S_K in $\mathcal{H}_1$, respectively. Then the adjoint, Friedrichs extension, and Krein–von Neumann extension of the nonnegative, closed, densely defined, symmetric operator USU^{-1} in $\mathcal{H}_2$ are given by*

$$[USU^{-1}]^* = US^*U^{-1}, \quad [USU^{-1}]_F = US_FU^{-1}, \quad [USU^{-1}]_K = US_KU^{-1} \tag{2.29}$$

in $\mathcal{H}_2$, respectively.

Proposition 2.4. *Let $J \subseteq \mathbb{N}$ be some countable index set and consider $\mathcal{H} = \bigoplus_{j\in J}\mathcal{H}_j$ and $S = \bigoplus_{j\in J} S_j$, where each S_j is a densely defined, closed, nonnegative operator in $\mathcal{H}_j$, $j \in J$. Denoting by $(S_j)_F$ and $(S_j)_K$ the Friedrichs and Krein–von Neumann extension of S_j in $\mathcal{H}_j$, $j \in J$, one infers*

$$S^* = \bigoplus_{j\in J} (S_j)^*, \quad S_F = \bigoplus_{j\in J} (S_j)_F, \quad S_K = \bigoplus_{j\in J} (S_j)_K. \tag{2.30}$$

The following is a consequence of a slightly more general result formulated in [16, Theorem 1]:

Proposition 2.5. *Let S be a densely defined, closed, nonnegative operator in $\mathcal{H}$. Then S_K, the Krein–von Neumann extension of S, has the property that*

$$\operatorname{dom}\big((S_K)^{1/2}\big) = \bigg\{u \in \mathcal{H}\,\bigg|\, \sup_{v\in\operatorname{dom}(S)} \frac{|(u,Sv)_{\mathcal{H}}|^2}{(v,Sv)_{\mathcal{H}}} < +\infty\bigg\}, \tag{2.31}$$

and

$$\big\|(S_K)^{1/2}u\big\|_{\mathcal{H}}^2 = \sup_{v\in\operatorname{dom}(S)} \frac{|(u,Sv)_{\mathcal{H}}|^2}{(v,Sv)_{\mathcal{H}}}, \quad u \in \operatorname{dom}\big((S_K)^{1/2}\big). \tag{2.32}$$

A word of explanation is in order here: Given $S \geq 0$ as in the statement of Proposition 2.5, the Cauchy–Schwarz-type inequality

$$|(u,Sv)_{\mathcal{H}}|^2 \leq (u,Su)_{\mathcal{H}}(v,Sv)_{\mathcal{H}}, \quad u,v \in \operatorname{dom}(S), \tag{2.33}$$

shows (due to the fact that $\operatorname{dom}(S) \hookrightarrow \mathcal{H}$ densely) that

$$u \in \operatorname{dom}(S) \text{ and } (u,Su)_{\mathcal{H}} = 0 \text{ imply } Su = 0. \tag{2.34}$$

Thus, whenever the denominator of the fractions appearing in (2.31), (2.32) vanishes, so does the numerator, and one interprets 0/0 as being zero in (2.31), (2.32).

We continue by recording an abstract result regarding the parametrization of all nonnegative self-adjoint extensions of a given strictly positive, densely defined, symmetric operator. The following results were developed from Krein [124], Višik [182], and Birman [37], by Grubb [94], [95]. Subsequent expositions are due to Faris [75, Sect. 15], Alonso and Simon [14] (in the present form, the next theorem appears in [89]), and Derkach and Malamud [65], [135]. We start by collecting our basic assumptions:

Hypothesis 2.6. *Suppose that S is a densely defined, symmetric, closed operator with nonzero deficiency indices in $\mathcal{H}$ that satisfies*

$$S \geq \varepsilon I_{\mathcal{H}} \text{ for some } \varepsilon > 0. \tag{2.35}$$

Theorem 2.7. *Suppose Hypothesis 2.6. Then there exists a one-to-one correspondence between nonnegative self-adjoint operators $0 \leq B : \operatorname{dom}(B) \subseteq \mathcal{W} \to \mathcal{W}$, $\overline{\operatorname{dom}(B)} = \mathcal{W}$, where $\mathcal{W}$ is a closed subspace of $\mathcal{N}_0 := \ker(S^*)$, and nonnegative self-adjoint extensions $S_{B,\mathcal{W}} \geq 0$ of S. More specifically, S_F is invertible, $S_F \geq \varepsilon I_{\mathcal{H}}$, and one has*

$$\begin{aligned} \operatorname{dom}(S_{B,\mathcal{W}}) &= \big\{f + (S_F)^{-1}(Bw+\eta) + w \,\big|\, \\ &\qquad f \in \operatorname{dom}(S),\, w \in \operatorname{dom}(B),\, \eta \in \mathcal{N}_0 \cap \mathcal{W}^{\perp}\big\}, \\ S_{B,\mathcal{W}} &= S^*|_{\operatorname{dom}(S_{B,\mathcal{W}})}, \end{aligned} \tag{2.36}$$

where $\mathcal{W}^\perp$ denotes the orthogonal complement of $\mathcal{W}$ in $\mathcal{N}_0$. In addition,

$$\operatorname{dom}\big((S_{B,\mathcal{W}})^{1/2}\big) = \operatorname{dom}\big((S_F)^{1/2}\big) \dotplus \operatorname{dom}\big(B^{1/2}\big), \tag{2.37}$$

$$\big\|(S_{B,\mathcal{W}})^{1/2}(u+g)\big\|_{\mathcal{H}}^2 = \big\|(S_F)^{1/2}u\big\|_{\mathcal{H}}^2 + \big\|B^{1/2}g\big\|_{\mathcal{H}}^2, \tag{2.38}$$
$$u \in \operatorname{dom}\big((S_F)^{1/2}\big),\ g \in \operatorname{dom}\big(B^{1/2}\big),$$

implying,

$$\ker(S_{B,\mathcal{W}}) = \ker(B). \tag{2.39}$$

Moreover,

$$B \le \widetilde{B} \ \textit{ implies } \ S_{B,\mathcal{W}} \le S_{\widetilde{B},\widetilde{\mathcal{W}}}, \tag{2.40}$$

where

$$\begin{aligned} &B\colon \operatorname{dom}(B) \subseteq \mathcal{W} \to \mathcal{W}, \quad \widetilde{B}\colon \operatorname{dom}\big(\widetilde{B}\big) \subseteq \widetilde{\mathcal{W}} \to \widetilde{\mathcal{W}}, \\ &\overline{\operatorname{dom}\big(\widetilde{B}\big)} = \widetilde{\mathcal{W}} \subseteq \mathcal{W} = \overline{\operatorname{dom}(B)}. \end{aligned} \tag{2.41}$$

In the above scheme, the Krein–von Neumann extension S_K of S corresponds to the choice $\mathcal{W} = \mathcal{N}_0$ and $B = 0$ (with $\operatorname{dom}(B) = \operatorname{dom}\big(B^{1/2}\big) = \mathcal{N}_0 = \ker(S^*)$). In particular, one thus recovers (2.10)*, and* (2.12)*, and also obtains*

$$\operatorname{dom}\big((S_K)^{1/2}\big) = \operatorname{dom}\big((S_F)^{1/2}\big) \dotplus \ker(S^*), \tag{2.42}$$

$$\big\|(S_K)^{1/2}(u+g)\big\|_{\mathcal{H}}^2 = \big\|(S_F)^{1/2}u\big\|_{\mathcal{H}}^2, \quad u \in \operatorname{dom}\big((S_F)^{1/2}\big),\ g \in \ker(S^*). \tag{2.43}$$

Finally, the Friedrichs extension S_F corresponds to the choice $\operatorname{dom}(B) = \{0\}$ (i.e., formally, $B \equiv \infty$), in which case one recovers (2.9).

The relation $B \le \widetilde{B}$ in the case where $\widetilde{\mathcal{W}} \subsetneqq \mathcal{W}$ requires an explanation: In analogy to (2.4) we mean

$$\big(|B|^{1/2}u, U_B|B|^{1/2}u\big)_{\mathcal{W}} \le \big(|\widetilde{B}|^{1/2}u, U_{\widetilde{B}}|\widetilde{B}|^{1/2}u\big)_{\mathcal{W}}, \quad u \in \operatorname{dom}\big(|\widetilde{B}|^{1/2}\big) \tag{2.44}$$

and (following [14]) we put

$$(|\widetilde{B}|^{1/2}u, U_{\widetilde{B}}|\widetilde{B}|^{1/2}u)_{\mathcal{W}} = \infty \ \text{ for } \ u \in \mathcal{W}\backslash \operatorname{dom}\big(|\widetilde{B}|^{1/2}\big). \tag{2.45}$$

For subsequent purposes we also note that under the assumptions on S in Hypothesis 2.6, one has

$$\dim(\ker(S^* - zI_{\mathcal{H}})) = \dim(\ker(S^*)) = \dim(\mathcal{N}_0) = \operatorname{def}(S), \quad z \in \mathbb{C}\backslash[\varepsilon,\infty). \tag{2.46}$$

The following result is a simple consequence of (2.10), (2.9), and (2.20), but since it seems not to have been explicitly stated in [124], we provide the short proof for completeness (see also [135, Remark 3]). First we recall that two self-adjoint extensions S_1 and S_2 of S are called *relatively prime* if $\operatorname{dom}(S_1) \cap \operatorname{dom}(S_2) = \operatorname{dom}(S)$.

Lemma 2.8. *Suppose Hypothesis* 2.6*. Then S_F and S_K are relatively prime, that is,*

$$\operatorname{dom}(S_F) \cap \operatorname{dom}(S_K) = \operatorname{dom}(S). \tag{2.47}$$

Proof. By (2.9) and (2.10) it suffices to prove that $\ker(S^*)\cap(S_F)^{-1}\ker(S^*)=\{0\}$. Let $f_0\in\ker(S^*)\cap(S_F)^{-1}\ker(S^*)$. Then $S^*f_0=0$ and $f_0=(S_F)^{-1}g_0$ for some $g_0\in\ker(S^*)$. Thus one concludes that $f_0\in\operatorname{dom}(S_F)$ and $S_Ff_0=g_0$. But $S_F=S^*|_{\operatorname{dom}(S_F)}$ and hence $g_0=S_Ff_0=S^*f_0=0$. Since $g_0=0$ one finally obtains $f_0=0$. □

Next, we consider a self-adjoint operator

$$T:\operatorname{dom}(T)\subseteq\mathcal{H}\to\mathcal{H},\quad T=T^*, \tag{2.48}$$

which is bounded from below, that is, there exists $\alpha\in\mathbb{R}$ such that

$$T\geq\alpha I_{\mathcal{H}}. \tag{2.49}$$

We denote by $\{E_T(\lambda)\}_{\lambda\in\mathbb{R}}$ the family of strongly right-continuous spectral projections of T, and introduce, as usual, $E_T((a,b))=E_T(b_-)-E_T(a)$, $E_T(b_-)=\operatorname{s-lim}_{\varepsilon\downarrow 0}E_T(b-\varepsilon)$, $-\infty\leq a<b$. In addition, we set

$$\mu_{T,j}:=\inf\big\{\lambda\in\mathbb{R}\,|\,\dim(\operatorname{ran}(E_T((-\infty,\lambda))))\geq j\big\},\quad j\in\mathbb{N}. \tag{2.50}$$

Then, for fixed $k\in\mathbb{N}$, either:

(i) $\mu_{T,k}$ is the kth eigenvalue of T counting multiplicity below the bottom of the essential spectrum, $\sigma_{\rm ess}(T)$, of T,

or,

(ii) $\mu_{T,k}$ is the bottom of the essential spectrum of T,

$$\mu_{T,k}=\inf\{\lambda\in\mathbb{R}\,|\,\lambda\in\sigma_{\rm ess}(T)\}, \tag{2.51}$$

and in that case $\mu_{T,k+\ell}=\mu_{T,k}$, $\ell\in\mathbb{N}$, and there are at most $k-1$ eigenvalues (counting multiplicity) of T below $\mu_{T,k}$.

We now record a basic result of M. Krein [124] with an important extension due to Alonso and Simon [14] and some additional results recently derived in [30]. For this purpose we introduce the *reduced Krein–von Neumann operator* $\widehat{S}_K$ in the Hilbert space (cf. (2.12))

$$\widehat{\mathcal{H}}=[\ker(S^*)]^\perp=\big[I_{\mathcal{H}}-P_{\ker(S^*)}\big]\mathcal{H}=\big[I_{\mathcal{H}}-P_{\ker(S_K)}\big]\mathcal{H}=[\ker(S_K)]^\perp, \tag{2.52}$$

by

$$\widehat{S}_K:=S_K|_{[\ker(S_K)]^\perp} \tag{2.53}$$

$$\begin{aligned}&=S_K[I_{\mathcal{H}}-P_{\ker(S_K)}]\ \text{ in } [I_{\mathcal{H}}-P_{\ker(S_K)}]\mathcal{H}\\ &=[I_{\mathcal{H}}-P_{\ker(S_K)}]S_K[I_{\mathcal{H}}-P_{\ker(S_K)}]\ \text{ in } [I_{\mathcal{H}}-P_{\ker(S_K)}]\mathcal{H},\end{aligned} \tag{2.54}$$

where $P_{\ker(S_K)}$ denotes the orthogonal projection onto $\ker(S_K)$ and we are alluding to the orthogonal direct sum decomposition of $\mathcal{H}$ into

$$\mathcal{H}=P_{\ker(S_K)}\mathcal{H}\oplus[I_{\mathcal{H}}-P_{\ker(S_K)}]\mathcal{H}. \tag{2.55}$$

We continue with the following elementary observation:

Lemma 2.9. *Assume Hypothesis* 2.6 *and let* $v \in \operatorname{dom}(S_K)$*. Then the decomposition,* $\operatorname{dom}(S_K) = \operatorname{dom}(S) \dotplus \ker(S^*)$ (*cf.* (2.10))*, leads to the following decomposition of* v*,*

$$v = (S_F)^{-1} S_K v + w, \quad \text{where } (S_F)^{-1} S_K v \in \operatorname{dom}(S) \text{ and } w \in \ker(S^*). \tag{2.56}$$

As a consequence,

$$\big(\widehat{S}_K\big)^{-1} = [I_{\mathcal{H}} - P_{\ker(S_K)}](S_F)^{-1}[I_{\mathcal{H}} - P_{\ker(S_K)}]. \tag{2.57}$$

We note that equation (2.57) was proved by Krein in his seminal paper [124] (cf. the proof of Theorem 26 in [124]). For a different proof of Krein's formula (2.57) and its generalization to the case of non-negative operators, see also [135, Corollary 5].

Theorem 2.10. *Suppose Hypothesis* 2.6*. Then,*

$$\varepsilon \leq \mu_{S_F,j} \leq \mu_{\widehat{S}_K,j}, \quad j \in \mathbb{N}. \tag{2.58}$$

In particular, if the Friedrichs extension S_F *of* S *has purely discrete spectrum, then, except possibly for* $\lambda = 0$*, the Krein–von Neumann extension* S_K *of* S *also has purely discrete spectrum in* $(0,\infty)$*, that is,*

$$\sigma_{\rm ess}(S_F) = \emptyset \text{ implies } \sigma_{\rm ess}(S_K)\backslash\{0\} = \emptyset. \tag{2.59}$$

In addition, let $p \in (0,\infty) \cup \{\infty\}$*, then*

$$\begin{aligned} &(S_F - z_0 I_{\mathcal{H}})^{-1} \in \mathcal{B}_p(\mathcal{H}) \text{ for some } z_0 \in \mathbb{C}\backslash[\varepsilon,\infty) \\ &\quad \text{implies } (S_K - zI_{\mathcal{H}})^{-1}[I_{\mathcal{H}} - P_{\ker(S_K)}] \in \mathcal{B}_p(\mathcal{H}) \text{ for all } z \in \mathbb{C}\backslash[\varepsilon,\infty). \end{aligned} \tag{2.60}$$

In fact, the $\ell^p(\mathbb{N})$*-based trace ideals* $\mathcal{B}_p(\mathcal{H})$ *of* $\mathcal{B}(\mathcal{H})$ *can be replaced by any two-sided symmetrically normed ideals of* $\mathcal{B}(\mathcal{H})$*.*

We note that (2.59) is a classical result of Krein [124], the more general fact (2.58) has not been mentioned explicitly in Krein's paper [124], although it immediately follows from the minimax principle and Krein's formula (2.57). On the other hand, in the special case $\operatorname{def}(S) < \infty$, Krein states an extension of (2.58) in his Remark 8.1 in the sense that he also considers self-adjoint extensions different from the Krein extension. Apparently, (2.58) in the context of infinite deficiency indices has first been proven by Alonso and Simon [14] by a somewhat different method. Relation (2.60) was recently proved in [30] for $p \in (0,\infty)$.

Concluding this section, we point out that a great variety of additional results for the Krein–von Neumann extension can be found, for instance, in [10, Sect. 109], [14], [16]–[18], [19, Chs. 9, 10], [20]–[25], [30], [49], [65], [66], [75, Part III], [76], [77], [82, Sect. 3.3], [89], [97], [102], [103], [105]–[108], [116], [117, Ch. 3], [126], [127], [148], [160], [168]–[170], [172], [178], [179], [181], and the references therein. We also mention the references [72]–[74] (these authors, apparently unaware of the work of von Neumann, Krein, Višhik, Birman, Grubb, Štrauss, etc., in this context, introduced the Krein Laplacian and called it the harmonic operator, see also [98]).

3. The abstract Krein–von Neumann extension and its connection to an abstract buckling problem

In this section we describe some results on the Krein–von Neumann extension which exhibit the latter as a natural object in elasticity theory by relating it to an abstract buckling problem. The results of this section appeared in [30].

We note that (2.59) is a classical result of Krein [124], the more general fact (2.58) has not been mentioned explicitly in Krein's paper [124], although it immediately follows from the minimax principle and Krein's formula (2.57). On the other hand, in the special case $\mathrm{def}(S) < \infty$, Krein states an extension of (2.58) in his Remark 8.1 in the sense that he also considers self-adjoint extensions different from the Krein extension. Apparently, (2.58) has first been proven by Alonso and Simon [14] by a somewhat different method. For a great variety of additional results on the Krein–von Neumann extension we refer to the very extensive list of references in [25], [29], and [106].

Next, we turn to the principal result of this section, the unitary equivalence of the inverse of the Krein–von Neumann extension (on the orthogonal complement of its kernel) of a densely defined, closed, operator S satisfying $S \geq \varepsilon I_{\mathcal{H}}$ for some $\varepsilon > 0$, in a complex separable Hilbert space $\mathcal{H}$ to an abstract buckling problem operator.

We start by introducing an abstract version of Proposition 1 in Grubb's paper [97] devoted to Krein–von Neumann extensions of even order elliptic differential operators on bounded domains:

Lemma 3.1. *Assume Hypothesis* 2.6 *and let* $\lambda \neq 0$. *Then there exists* $0 \neq v \in \mathrm{dom}(S_K)$ *with*

$$S_K v = \lambda v \tag{3.1}$$

if and only if there exists $0 \neq u \in \mathrm{dom}(S^*S)$ *such that*

$$S^*Su = \lambda Su. \tag{3.2}$$

In particular, the solutions v *of* (3.1) *are in one-to-one correspondence with the solutions* u *of* (3.2) *given by the formulas*

$$u = (S_F)^{-1} S_K v, \tag{3.3}$$

$$v = \lambda^{-1} Su. \tag{3.4}$$

Of course, since $S_K \geq 0$, *any* $\lambda \neq 0$ *in* (3.1) *and* (3.2) *necessarily satisfies* $\lambda > 0$.

Proof. Let $S_K v = \lambda v$, $v \in \mathrm{dom}(S_K)$, $\lambda \neq 0$, and $v = u + w$, with $u \in \mathrm{dom}(S)$ and $w \in \ker(S^*)$. Then,

$$S_K v = \lambda v \Longleftrightarrow v = \lambda^{-1} S_K v = \lambda^{-1} S_K u = \lambda^{-1} Su. \tag{3.5}$$

Moreover, $u = 0$ implies $v = 0$ and clearly $v = 0$ implies $u = w = 0$, hence $v \neq 0$ if and only if $u \neq 0$. In addition, $u = (S_F)^{-1} S_K v$ by (2.56). Finally,

$$\begin{aligned} &\lambda w = Su - \lambda u \in \ker(S^*) \ \text{ implies} \\ &0 = \lambda S^* w = S^*(Su - \lambda u) = S^*Su - \lambda S^* u = S^*Su - \lambda Su. \end{aligned} \tag{3.6}$$

Conversely, suppose $u \in \operatorname{dom}(S^*S)$ and $S^*Su = \lambda Su$, $\lambda \neq 0$. Introducing $v = \lambda^{-1}Su$, then $v \in \operatorname{dom}(S^*)$ and

$$S^*v = \lambda^{-1}S^*Su = Su = \lambda v. \tag{3.7}$$

Noticing that

$$S^*Su = \lambda Su = \lambda S^*u \text{ implies } S^*(S - \lambda I_{\mathcal{H}})u = 0, \tag{3.8}$$

and hence $(S - \lambda I_{\mathcal{H}})u \in \ker(S^*)$, rewriting v as

$$v = u + \lambda^{-1}(S - \lambda I_{\mathcal{H}})u \tag{3.9}$$

then proves that also $v \in \operatorname{dom}(S_K)$, using (2.10) again. □

Due to Example 3.5 and Remark 3.6 at the end of this section, we will call the linear pencil eigenvalue problem $S^*Su = \lambda Su$ in (3.2) the *abstract buckling problem* associated with the Krein–von Neumann extension S_K of S.

Next, we turn to a variational formulation of the correspondence between the inverse of the reduced Krein extension $\widehat{S}_K$ and the abstract buckling problem in terms of appropriate sesquilinear forms by following the treatment of Kozlov [118]–[120] in the context of elliptic partial differential operators. This will then lead to an even stronger connection between the Krein–von Neumann extension S_K of S and the associated abstract buckling eigenvalue problem (3.2), culminating in a unitary equivalence result in Theorem 3.4.

Given the operator S, we introduce the following sesquilinear forms in $\mathcal{H}$,

$$a(u,v) = (Su, Sv)_{\mathcal{H}}, \quad u,v \in \operatorname{dom}(a) = \operatorname{dom}(S), \tag{3.10}$$

$$b(u,v) = (u, Sv)_{\mathcal{H}}, \qquad u,v \in \operatorname{dom}(b) = \operatorname{dom}(S). \tag{3.11}$$

Then S being densely defined and closed implies that the sesquilinear form a shares these properties and (2.35) implies its boundedness from below,

$$a(u,u) \geq \varepsilon^2 \|u\|_{\mathcal{H}}^2, \quad u \in \operatorname{dom}(S). \tag{3.12}$$

Thus, one can introduce the Hilbert space $\mathcal{W} = (\operatorname{dom}(S), (\cdot,\cdot)_{\mathcal{W}})$ with associated scalar product

$$(u,v)_{\mathcal{W}} = a(u,v) = (Su, Sv)_{\mathcal{H}}, \quad u,v \in \operatorname{dom}(S). \tag{3.13}$$

In addition, we denote by $\iota_{\mathcal{W}}$ the continuous embedding operator of $\mathcal{W}$ into $\mathcal{H}$,

$$\iota_{\mathcal{W}} : \mathcal{W} \hookrightarrow \mathcal{H}. \tag{3.14}$$

Hence we will use the notation

$$(w_1, w_2)_{\mathcal{W}} = a(\iota_{\mathcal{W}} w_1, \iota_{\mathcal{W}} w_2) = (S\iota_{\mathcal{W}} w_1, S\iota_{\mathcal{W}} w_2)_{\mathcal{H}}, \quad w_1, w_2 \in \mathcal{W}, \tag{3.15}$$

in the following.

Given the sesquilinear forms a and b and the Hilbert space $\mathcal{W}$, we next define the operator T in $\mathcal{W}$ by

$$\begin{aligned}(w_1, Tw_2)_{\mathcal{W}} &= a(\iota_{\mathcal{W}} w_1, \iota_{\mathcal{W}} T w_2) = (S\iota_{\mathcal{W}} w_1, S\iota_{\mathcal{W}} T w_2)_{\mathcal{H}} \\ &= b(\iota_{\mathcal{W}} w_1, \iota_{\mathcal{W}} w_2) = (\iota_{\mathcal{W}} w_1, S\iota_{\mathcal{W}} w_2)_{\mathcal{H}}, \quad w_1, w_2 \in \mathcal{W}.\end{aligned} \tag{3.16}$$

(In contrast to the informality of our introduction, we now explicitly write the embedding operator $\iota_{\mathcal{W}}$.) One verifies that T is well defined and that

$$|(w_1, Tw_2)_{\mathcal{W}}| \leq \|\iota_{\mathcal{W}} w_1\|_{\mathcal{H}} \|S\iota_{\mathcal{W}} w_2\|_{\mathcal{H}} \leq \varepsilon^{-1} \|w_1\|_{\mathcal{W}} \|w_2\|_{\mathcal{W}}, \quad w_1, w_2 \in \mathcal{W}, \tag{3.17}$$

and hence that

$$0 \leq T = T^* \in \mathcal{B}(\mathcal{W}), \quad \|T\|_{\mathcal{B}(\mathcal{W})} \leq \varepsilon^{-1}. \tag{3.18}$$

For reasons to become clear at the end of this section, we will call T the *abstract buckling problem operator* associated with the Krein–von Neumann extension S_K of S.

Next, recalling the notation $\widehat{\mathcal{H}} = [\ker(S^*)]^{\perp} = \big[I_{\mathcal{H}} - P_{\ker(S^*)}\big]\mathcal{H}$ (cf. (2.52)), we introduce the operator

$$\widehat{S} : \begin{cases} \mathcal{W} \to \widehat{\mathcal{H}}, \\ w \mapsto S\iota_{\mathcal{W}} w, \end{cases} \tag{3.19}$$

and note that

$$\operatorname{ran}\big(\widehat{S}\big) = \operatorname{ran}(S) = \widehat{\mathcal{H}}, \tag{3.20}$$

since $S \geq \varepsilon I_{\mathcal{H}}$ for some $\varepsilon > 0$ and S is closed in $\mathcal{H}$ (see, e.g., [185, Theorem 5.32]). In fact, one has the following result:

Lemma 3.2. *Assume Hypothesis* 2.6*. Then* $\widehat{S} \in \mathcal{B}(\mathcal{W}, \widehat{\mathcal{H}})$ *maps* $\mathcal{W}$ *unitarily onto* $\widehat{\mathcal{H}}$*.*

Proof. Clearly $\widehat{S}$ is an isometry since

$$\big\|\widehat{S}w\big\|_{\widehat{\mathcal{H}}} = \|S\iota_{\mathcal{W}} w\|_{\mathcal{H}} = \|w\|_{\mathcal{W}}, \quad w \in \mathcal{W}. \tag{3.21}$$

Since $\operatorname{ran}\big(\widehat{S}\big) = \widehat{\mathcal{H}}$ by (3.20), $\widehat{S}$ is unitary. □

Next we recall the definition of the reduced Krein–von Neumann operator $\widehat{S}_K$ in $\widehat{\mathcal{H}}$ defined in (2.54), the fact that $\ker(S^*) = \ker(S_K)$ by (2.12), and state the following auxiliary result:

Lemma 3.3. *Assume Hypothesis* 2.6*. Then the map*

$$\big[I_{\mathcal{H}} - P_{\ker(S^*)}\big] : \operatorname{dom}(S) \to \operatorname{dom}\big(\widehat{S}_K\big) \tag{3.22}$$

is a bijection. In addition, we note that

$$\begin{aligned} \big[I_{\mathcal{H}} - P_{\ker(S^*)}\big] S_K u &= S_K \big[I_{\mathcal{H}} - P_{\ker(S^*)}\big] u = \widehat{S}_K \big[I_{\mathcal{H}} - P_{\ker(S^*)}\big] u \\ &= \big[I_{\mathcal{H}} - P_{\ker(S^*)}\big] S u = S u \in \widehat{\mathcal{H}}, \quad u \in \operatorname{dom}(S). \end{aligned} \tag{3.23}$$

Proof. Let $u \in \operatorname{dom}(S)$, then $\ker(S^*) = \ker(S_K)$ implies that $\big[I_{\mathcal{H}} - P_{\ker(S^*)}\big]u \in \operatorname{dom}(S_K)$ and of course $\big[I_{\mathcal{H}} - P_{\ker(S^*)}\big]u \in \operatorname{dom}\big(\widehat{S}_K\big)$. To prove injectivity of the map (3.22) it suffices to assume $v \in \operatorname{dom}(S)$ and $\big[I_{\mathcal{H}} - P_{\ker(S^*)}\big]v = 0$. Then $\operatorname{dom}(S) \ni v = P_{\ker(S^*)} v \in \ker(S^*)$ yields $v = 0$ as $\operatorname{dom}(S) \cap \ker(S^*) = \{0\}$. To prove surjectivity of the map (3.22) we suppose $u \in \operatorname{dom}\big(\widehat{S}_K\big)$. The decomposition, $u = f + g$ with $f \in \operatorname{dom}(S)$ and $g \in \ker(S^*)$, then yields

$$u = \big[I_{\mathcal{H}} - P_{\ker(S^*)}\big]u = \big[I_{\mathcal{H}} - P_{\ker(S^*)}\big]f \in \big[I_{\mathcal{H}} - P_{\ker(S^*)}\big] \operatorname{dom}(S) \tag{3.24}$$

and hence proves surjectivity of (3.22).

Equation (3.23) is clear from

$$S_K\big[I_{\mathcal{H}} - P_{\ker(S^*)}\big] = \big[I_{\mathcal{H}} - P_{\ker(S^*)}\big]S_K \tag{3.25}$$
$$= \big[I_{\mathcal{H}} - P_{\ker(S^*)}\big]S_K\big[I_{\mathcal{H}} - P_{\ker(S^*)}\big]. \qquad \square$$

Continuing, we briefly recall the polar decomposition of S,

$$S = U_S|S|, \tag{3.26}$$

with

$$|S| = (S^*S)^{1/2} \geq \varepsilon I_{\mathcal{H}},\ \varepsilon > 0, \quad U_S \in \mathcal{B}\big(\mathcal{H}, \widehat{\mathcal{H}}\big) \text{ is unitary.} \tag{3.27}$$

At this point we are in position to state our principal unitary equivalence result:

Theorem 3.4. *Assume Hypothesis* 2.6*. Then the inverse of the reduced Krein–von Neumann extension* $\widehat{S}_K$ *in* $\widehat{\mathcal{H}} = \big[I_{\mathcal{H}} - P_{\ker(S^*)}\big]\mathcal{H}$ *and the abstract buckling problem operator* T *in* $\mathcal{W}$ *are unitarily equivalent, in particular,*

$$\big(\widehat{S}_K\big)^{-1} = \widehat{S}T(\widehat{S})^{-1}. \tag{3.28}$$

Moreover, one has

$$\big(\widehat{S}_K\big)^{-1} = U_S\big[|S|^{-1}S|S|^{-1}\big](U_S)^{-1}, \tag{3.29}$$

where $U_S \in \mathcal{B}\big(\mathcal{H}, \widehat{\mathcal{H}}\big)$ *is the unitary operator in the polar decomposition* (3.26) *of* S *and the operator* $|S|^{-1}S|S|^{-1} \in \mathcal{B}(\mathcal{H})$ *is self-adjoint in* $\mathcal{H}$*.*

Proof. Let $w_1, w_2 \in \mathcal{W}$. Then,

$$\begin{aligned}
&\big(w_1, \big(\widehat{S}\big)^{-1}\big(\widehat{S}_K\big)^{-1}\widehat{S}w_2\big)_{\mathcal{W}} = \big(\widehat{S}w_1, \big(\widehat{S}_K\big)^{-1}\widehat{S}w_2\big)_{\widehat{\mathcal{H}}} \\
&\quad = \big(\big(\widehat{S}_K\big)^{-1}\widehat{S}w_1, \widehat{S}w_2\big)_{\widehat{\mathcal{H}}} = \big(\big(\widehat{S}_K\big)^{-1}S\iota_{\mathcal{W}}w_1, \widehat{S}w_2\big)_{\widehat{\mathcal{H}}} \\
&\quad = \big(\big(\widehat{S}_K\big)^{-1}\big[I_{\mathcal{H}} - P_{\ker(S^*)}\big]S\iota_{\mathcal{W}}w_1, \widehat{S}w_2\big)_{\widehat{\mathcal{H}}} \quad \text{by (3.23)} \\
&\quad = \big(\big(\widehat{S}_K\big)^{-1}\widehat{S}_K\big[I_{\mathcal{H}} - P_{\ker(S^*)}\big]\iota_{\mathcal{W}}w_1, \widehat{S}w_2\big)_{\widehat{\mathcal{H}}} \quad \text{again by (3.23)} \\
&\quad = \big(\big[I_{\mathcal{H}} - P_{\ker(S^*)}\big]\iota_{\mathcal{W}}w_1, \widehat{S}w_2\big)_{\widehat{\mathcal{H}}} \\
&\quad = \big(\iota_{\mathcal{W}}w_1, S\iota_{\mathcal{W}}w_2\big)_{\mathcal{H}} \\
&\quad = \big(w_1, Tw_2\big)_{\mathcal{W}} \quad \text{by definition of } T \text{ in (3.16)},
\end{aligned} \tag{3.30}$$

yields (3.28). In addition one verifies that

$$\begin{aligned}
\big(\widehat{S}w_1, \big(\widehat{S}_K\big)^{-1}\widehat{S}w_2\big)_{\widehat{\mathcal{H}}} &= \big(w_1, Tw_2\big)_{\mathcal{W}} \\
&= \big(\iota_{\mathcal{W}}w_1, S\iota_{\mathcal{W}}w_2\big)_{\mathcal{H}} \\
&= \big(|S|^{-1}|S|\iota_{\mathcal{W}}w_1, S|S|^{-1}|S|\iota_{\mathcal{W}}w_2\big)_{\mathcal{H}} \\
&= \big(|S|\iota_{\mathcal{W}}w_1, \big[|S|^{-1}S|S|^{-1}\big]|S|\iota_{\mathcal{W}}w_2\big)_{\mathcal{H}} \\
&= \big((U_S)^*S\iota_{\mathcal{W}}w_1, \big[|S|^{-1}S|S|^{-1}\big](U_S)^*S\iota_{\mathcal{W}}w_2\big)_{\mathcal{H}}
\end{aligned}$$

$$
\begin{aligned}
&= \big(S\iota_{\mathcal{W}} w_1, U_S\big[|S|^{-1}S|S|^{-1}\big](U_S)^* S\iota_{\mathcal{W}} w_2\big)_{\mathcal{H}} \\
&= \big(\widehat{S} w_1, U_S\big[|S|^{-1}S|S|^{-1}\big](U_S)^* \widehat{S} w_2\big)_{\widehat{\mathcal{H}}}, \qquad (3.31)
\end{aligned}
$$

where we used $|S| = (U_S)^* S$. □

Equation (3.29) is of course motivated by rewriting the abstract linear pencil buckling eigenvalue problem (3.2), $S^*Su = \lambda Su$, $\lambda \neq 0$, in the form

$$
\lambda^{-1} S^*Su = \lambda^{-1}(S^*S)^{1/2}\big[(S^*S)^{1/2}u\big] = S(S^*S)^{-1/2}\big[(S^*S)^{1/2}u\big] \qquad (3.32)
$$

and hence in the form of a standard eigenvalue problem

$$
|S|^{-1}S|S|^{-1}w = \lambda^{-1}w, \quad \lambda \neq 0, \quad w = |S|u. \qquad (3.33)
$$

We conclude this section with a concrete example discussed explicitly in Grubb [97] (see also [94]–[96] for necessary background) and make the explicit connection with the buckling problem. It was this example which greatly motivated the abstract results in this note:

Example 3.5. ([97].) Let $\mathcal{H} = L^2(\Omega; d^n x)$, with $\Omega \subset \mathbb{R}^n$, $n \geq 2$, open, bounded, and smooth (i.e., with a smooth boundary $\partial\Omega$), and consider the minimal operator realization S of the differential expression $\mathscr{S}$ in $L^2(\Omega; d^n x)$, defined by

$$
\begin{aligned}
&Su = \mathscr{S}u, \qquad (3.34) \\
&u \in \operatorname{dom}(S) = H_0^{2m}(\Omega) = \big\{v \in H^{2m}(\Omega) \,\big|\, \gamma_k v = 0,\, 0 \leq k \leq 2m-1\big\}, \quad m \in \mathbb{N},
\end{aligned}
$$

where

$$
\mathscr{S} = \sum_{0 \leq |\alpha| \leq 2m} a_\alpha(\cdot) D^\alpha, \qquad (3.35)
$$

$$
D^\alpha = (-i\partial/\partial x_1)^{\alpha_1} \cdots (-i\partial/\partial x_n)^{\alpha_n}, \quad \alpha = (\alpha_1, \dots, \alpha_n) \in \mathbb{N}_0^n, \qquad (3.36)
$$

$$
a_\alpha(\cdot) \in C^\infty(\overline{\Omega}), \quad C^\infty(\overline{\Omega}) = \bigcap_{k \in \mathbb{N}_0} C^k(\overline{\Omega}), \qquad (3.37)
$$

and the coefficients a_α are chosen such that S is symmetric in $L^2(\mathbb{R}^n; d^n x)$, that is, the differential expression $\mathscr{S}$ is formally self-adjoint,

$$
(\mathscr{S}u, v)_{L^2(\mathbb{R}^n; d^n x)} = (u, \mathscr{S}v)_{L^2(\mathbb{R}^n; d^n x)}, \quad u, v \in C_0^\infty(\Omega), \qquad (3.38)
$$

and $\mathscr{S}$ is strongly elliptic, that is, for some $c > 0$,

$$
\operatorname{Re}\bigg(\sum_{|\alpha| = 2m} a_\alpha(x)\xi^\alpha\bigg) \geq c|\xi|^{2m}, \quad x \in \overline{\Omega},\ \xi \in \mathbb{R}^n. \qquad (3.39)
$$

In addition, we assume that $S \geq \varepsilon I_{L^2(\Omega; d^n x)}$ for some $\varepsilon > 0$. The trace operators γ_k are defined as follows: Consider

$$
\mathring{\gamma}_k : \begin{cases} C^\infty(\overline{\Omega}) \to C^\infty(\partial\Omega) \\ u \mapsto (\partial_n^k u)|_{\partial\Omega}, \end{cases} \qquad (3.40)
$$

with ∂_n denoting the interior normal derivative. The map $\mathring{\gamma}$ then extends by continuity to a bounded operator

$$\gamma_k : H^s(\Omega) \to H^{s-k-(1/2)}(\partial\Omega), \quad s > k + (1/2), \tag{3.41}$$

in addition, the map

$$\gamma^{(r)} = (\gamma_0, \dots, \gamma_r) : H^s(\Omega) \to \prod_{k=0}^{r} H^{s-k-(1/2)}(\partial\Omega), \quad s > r + (1/2), \tag{3.42}$$

satisfies

$$\ker\big(\gamma^{(r)}\big) = H_0^s(\Omega), \quad \operatorname{ran}\big(\gamma^{(r)}\big) = \prod_{k=0}^{r} H^{s-k-(1/2)}(\partial\Omega). \tag{3.43}$$

Then S^*, the maximal operator realization of $\mathscr{S}$ in $L^2(\Omega; d^n x)$, is given by

$$S^* u = \mathscr{S} u, \quad u \in \operatorname{dom}(S^*) = \big\{v \in L^2(\Omega; d^n x) \,\big|\, \mathscr{S} v \in L^2(\Omega; d^n x)\big\}, \tag{3.44}$$

and S_F is characterized by

$$S_F u = \mathscr{S} u, \quad u \in \operatorname{dom}(S_F) = \big\{v \in H^{2m}(\Omega) \,\big|\, \gamma_k v = 0,\, 0 \le k \le m-1\big\}. \tag{3.45}$$

The Krein–von Neumann extension S_K of S then has the domain

$$\operatorname{dom}(S_K) = H_0^{2m}(\Omega) \dotplus \ker(S^*), \quad \dim(\ker(S^*)) = \infty, \tag{3.46}$$

and elements $u \in \operatorname{dom}(S_K)$ satisfy the nonlocal boundary condition

$$\gamma_N u - P_{\gamma_D, \gamma_N} \gamma_D u = 0, \tag{3.47}$$

$$\gamma_D u = (\gamma_0 u, \dots, \gamma_{m-1} u), \quad \gamma_N u = (\gamma_m u, \dots, \gamma_{2m-1} u), \quad u \in \operatorname{dom}(S_K), \tag{3.48}$$

where

$$\begin{aligned} P_{\gamma_D, \gamma_N} &= \gamma_N \gamma_Z^{-1} : \prod_{k=0}^{m-1} H^{s-k-(1/2)}(\partial\Omega) \\ &\quad \to \prod_{j=m}^{2m-1} H^{s-j-(1/2)}(\partial\Omega) \text{ continuously for all } s \in \mathbb{R}, \end{aligned} \tag{3.49}$$

and γ_Z^{-1} denotes the inverse of the isomorphism γ_Z given by

$$\gamma_D : Z^s_{\mathscr{S}} \to \prod_{k=0}^{m-1} H^{s-k-(1/2)}(\partial\Omega), \tag{3.50}$$

$$\begin{aligned} Z^s_{\mathscr{S}} = \big\{u \in H^s(\Omega) \,\big|\, \mathscr{S} u = 0 \text{ in } \Omega \text{ in the sense of} \\ \text{distributions in } \mathcal{D}'(\Omega)\big\}, \quad s \in \mathbb{R}. \end{aligned} \tag{3.51}$$

Moreover one has

$$\big(\widehat{S}\big)^{-1} = \iota_{\mathcal{W}} [I_{\mathcal{H}} - P_{\gamma_D, \gamma_N} \gamma_D] \big(\widehat{S}_K\big)^{-1}, \tag{3.52}$$

since $[I_{\mathcal{H}} - P_{\gamma_D, \gamma_N} \gamma_D] \operatorname{dom}(S_K) \subseteq \operatorname{dom}(S)$ and $S[I_{\mathcal{H}} - P_{\gamma_D, \gamma_N} \gamma_D] v = \lambda v$, $v \in \operatorname{dom}(S_K)$.

As discussed in detail in Grubb [97],

$$\sigma_{\mathrm{ess}}(S_K) = \{0\}, \quad \sigma(S_K) \cap (0,\infty) = \sigma_{\mathrm{d}}(S_K) \tag{3.53}$$

and the nonzero (and hence discrete) eigenvalues of S_K satisfy a Weyl-type asymptotics. The connection to a higher-order buckling eigenvalue problem established by Grubb then reads

$$\text{There exists } 0 \neq v \in \mathrm{dom}(S_K) \text{ satisfying } \mathscr{S} v = \lambda v \text{ in } \Omega, \quad \lambda \neq 0 \tag{3.54}$$

if and only if

$$\text{there exists } 0 \neq u \in C^\infty(\overline{\Omega}) \text{ such that } \begin{cases} \mathscr{S}^2 u = \lambda \mathscr{S} u \text{ in } \Omega, \quad \lambda \neq 0, \\ \gamma_k u = 0, \ 0 \leq k \leq 2m-1, \end{cases} \tag{3.55}$$

where the solutions v of (3.54) are in one-to-one correspondence with the solutions u of (3.55) via

$$u = S_F^{-1} \mathscr{S} v, \quad v = \lambda^{-1} \mathscr{S} u. \tag{3.56}$$

Since S_F has purely discrete spectrum in Example 3.5, we note that Theorem 2.10 applies in this case.

Remark 3.6. In the particular case $m = 1$ and $\mathscr{S} = -\Delta$, the linear pencil eigenvalue problem (3.55) (i.e., the concrete analog of the abstract buckling eigenvalue problem $S^*Su = \lambda Su$, $\lambda \neq 0$, in (3.2)), then yields the *buckling of a clamped plate problem*,

$$(-\Delta)^2 u = \lambda(-\Delta)u \text{ in } \Omega, \quad \lambda \neq 0, \ u \in H_0^2(\Omega), \tag{3.57}$$

as distributions in $H^{-2}(\Omega)$. Here we used the fact that for any nonempty bounded open set $\Omega \subset \mathbb{R}^n$, $n \in \mathbb{N}$, $n \geq 2$, $(-\Delta)^m \in \mathcal{B}\big(H^k(\Omega), H^{k-2m}(\Omega)\big)$, $k \in \mathbb{Z}$, $m \in \mathbb{N}$. In addition, if Ω is a Lipschitz domain, then one has that $-\Delta\colon H_0^1(\Omega) \to H^{-1}(\Omega)$ is an isomorphism and similarly, $(-\Delta)^2\colon H_0^2(\Omega) \to H^{-2}(\Omega)$ is an isomorphism. (For the natural norms on $H^k(\Omega)$, $k \in \mathbb{Z}$, see, e.g., [142, p. 73–75].) We refer, for instance, to [36, Sect. 4.3B] for a derivation of (3.57) from the fourth-order system of quasilinear von Kármán partial differential equations. To be precise, (3.57) should also be considered in the special case $n = 2$.

Remark 3.7. We emphasize that the smoothness hypotheses on $\partial\Omega$ can be relaxed in the special case of the second-order Schrödinger operator associated with the differential expression $-\Delta + V$, where $V \in L^\infty(\Omega; d^n x)$ is real valued: Following the treatment of self-adjoint extensions of $S = \overline{(-\Delta + V)|_{C_0^\infty(\Omega)}}$ on quasi-convex domains Ω introduced in [89], and recalled in Section 6, the case of the Krein–von Neumann extension S_K of S on such quasi-convex domains (which are close to minimally smooth) is treated in great detail in [29] and in the remainder of this survey (cf. Section 7). In particular, a Weyl-type asymptotics of the associated (nonzero) eigenvalues of S_K, to be discussed in Section 9, has been proven in [29]. In the higher-order smooth case described in Example 3.5, a Weyl-type asymptotic for the nonzero eigenvalues of S_K has been proven by Grubb [97] in 1983.

4. Trace theory in Lipschitz domains

In this section we shall review material pertaining to analysis in Lipschitz domains, starting with Dirichlet and Neumann boundary traces in Subsection 4.1, and then continuing with a brief survey of perturbed Dirichlet and Neumann Laplacians in Subsection 4.2.

4.1. Dirichlet and Neumann traces in Lipschitz domains

The goal of this subsection is to introduce the relevant material pertaining to Sobolev spaces $H^s(\Omega)$ and $H^r(\partial\Omega)$ corresponding to subdomains Ω of $\mathbb{R}^n$, $n \in \mathbb{N}$, and discuss various trace results.

Before we focus primarily on bounded Lipschitz domains (we recall our use of "domain" as an open subset of $\mathbb{R}^n$, without any connectivity hypotheses), we briefly recall some basic facts in connection with Sobolev spaces corresponding to open sets $\Omega \subseteq \mathbb{R}^n$, $n \in \mathbb{N}$: For an arbitrary $m \in \mathbb{N} \cup \{0\}$, we follow the customary way of defining L^2-Sobolev spaces of order $\pm m$ in Ω as

$$H^m(\Omega) := \big\{u \in L^2(\Omega; d^n x) \,\big|\, \partial^\alpha u \in L^2(\Omega; d^n x),\, 0 \leq |\alpha| \leq m\big\}, \tag{4.1}$$

$$H^{-m}(\Omega) := \bigg\{u \in \mathcal{D}'(\Omega) \,\bigg|\, u = \sum_{0 \leq |\alpha| \leq m} \partial^\alpha u_\alpha, \text{ with } u_\alpha \in L^2(\Omega; d^n x),\, 0 \leq |\alpha| \leq m\bigg\}, \tag{4.2}$$

equipped with natural norms (cf., e.g., [2, Ch. 3], [137, Ch. 1]). Here $\mathcal{D}'(\Omega)$ denotes the usual set of distributions on $\Omega \subseteq \mathbb{R}^n$. Then we set

$$H_0^m(\Omega) := \text{the closure of } C_0^\infty(\Omega) \text{ in } H^m(\Omega), \quad m \in \mathbb{N} \cup \{0\}. \tag{4.3}$$

As is well known, all three spaces above are Banach, reflexive and, in addition,

$$\big(H_0^m(\Omega)\big)^* = H^{-m}(\Omega). \tag{4.4}$$

Again, see, for instance, [2, Ch. 3], [137, Ch. 1].

We recall that an open, nonempty set $\Omega \subseteq \mathbb{R}^n$ is called a *Lipschitz domain* if the following property holds: There exists an open covering $\{\mathcal{O}_j\}_{1 \leq j \leq N}$ of the boundary $\partial\Omega$ of Ω such that for every $j \in \{1, \dots, N\}$, $\mathcal{O}_j \cap \Omega$ coincides with the portion of $\mathcal{O}_j$ lying in the over-graph of a Lipschitz function $\varphi_j : \mathbb{R}^{n-1} \to \mathbb{R}$ (considered in a new system of coordinates obtained from the original one via a rigid motion). The number $\max\{\|\nabla\varphi_j\|_{L^\infty(\mathbb{R}^{n-1}; d^{n-1}x')^{n-1}} \,|\, 1 \leq j \leq N\}$ is said to represent the *Lipschitz character* of Ω.

The classical theorem of Rademacher on almost everywhere differentiability of Lipschitz functions ensures that for any Lipschitz domain Ω, the surface measure $d^{n-1}\omega$ is well defined on $\partial\Omega$ and that there exists an outward pointing normal vector ν at almost every point of $\partial\Omega$.

As regards L^2-based Sobolev spaces of fractional order $s \in \mathbb{R}$, on arbitrary Lipschitz domains $\Omega \subseteq \mathbb{R}^n$, we introduce

$$H^s(\mathbb{R}^n) := \left\{ U \in \mathcal{S}'(\mathbb{R}^n) \,\middle|\, \|U\|^2_{H^s(\mathbb{R}^n)} = \int_{\mathbb{R}^n} d^n\xi \, \big|\widehat{U}(\xi)\big|^2 \big(1 + |\xi|^{2s}\big) < \infty \right\}, \tag{4.5}$$

$$H^s(\Omega) := \big\{ u \in \mathcal{D}'(\Omega) \,\big|\, u = U|_\Omega \text{ for some } U \in H^s(\mathbb{R}^n) \big\} = R_\Omega \, H^s(\mathbb{R}^n), \tag{4.6}$$

where R_Ω denotes the restriction operator (i.e., $R_\Omega \, U = U|_\Omega$, $U \in H^s(\mathbb{R}^n)$), $\mathcal{S}'(\mathbb{R}^n)$ is the space of tempered distributions on $\mathbb{R}^n$, and $\widehat{U}$ denotes the Fourier transform of $U \in \mathcal{S}'(\mathbb{R}^n)$. These definitions are consistent with (4.1), (4.2). Next, retaining that $\Omega \subseteq \mathbb{R}^n$ is an arbitrary Lipschitz domain, we introduce

$$H^s_0(\Omega) := \big\{ u \in H^s(\mathbb{R}^n) \,\big|\, \mathrm{supp}(u) \subseteq \overline{\Omega} \big\}, \quad s \in \mathbb{R}, \tag{4.7}$$

equipped with the natural norm induced by $H^s(\mathbb{R}^n)$. The space $H^s_0(\Omega)$ is reflexive, being a closed subspace of $H^s(\mathbb{R}^n)$. Finally, we introduce for all $s \in \mathbb{R}$,

$$\mathring{H}^s(\Omega) = \text{the closure of } C^\infty_0(\Omega) \text{ in } H^s(\Omega), \tag{4.8}$$

$$H^s_z(\Omega) = R_\Omega \, H^s_0(\Omega). \tag{4.9}$$

Assuming from now on that $\Omega \subset \mathbb{R}^n$ is a Lipschitz domain with a compact boundary, we recall the existence of a universal linear extension operator $E_\Omega : \mathcal{D}'(\Omega) \to \mathcal{S}'(\mathbb{R}^n)$ such that $E_\Omega : H^s(\Omega) \to H^s(\mathbb{R}^n)$ is bounded for all $s \in \mathbb{R}$, and $R_\Omega E_\Omega = I_{H^s(\Omega)}$ (cf. [163]). If $\widetilde{C^\infty_0(\Omega)}$ denotes the set of $C^\infty_0(\Omega)$-functions extended to all of $\mathbb{R}^n$ by setting functions zero outside of Ω, then for all $s \in \mathbb{R}$, $\widetilde{C^\infty_0(\Omega)} \hookrightarrow H^s_0(\Omega)$ densely.

Moreover, one has

$$\big(H^s_0(\Omega)\big)^* = H^{-s}(\Omega), \quad s \in \mathbb{R}. \tag{4.10}$$

(cf., e.g., [113]) consistent with (4.3), and also,

$$\big(H^s(\Omega)\big)^* = H^{-s}_0(\Omega), \quad s \in \mathbb{R}, \tag{4.11}$$

in particular, $H^s(\Omega)$ is a reflexive Banach space. We shall also use the fact that for a Lipschitz domain $\Omega \subset \mathbb{R}^n$ with compact boundary, the space $\mathring{H}^s(\Omega)$ satisfies

$$\mathring{H}^s(\Omega) = H^s_z(\Omega) \text{ if } s > -1/2, \ s \notin \big\{\tfrac{1}{2} + \mathbb{N}_0\big\}. \tag{4.12}$$

For a Lipschitz domain $\Omega \subseteq \mathbb{R}^n$ with compact boundary it is also known that

$$\big(H^s(\Omega)\big)^* = H^{-s}(\Omega), \quad -1/2 < s < 1/2. \tag{4.13}$$

See [176] for this and other related properties. Throughout this survey, we agree to use the *adjoint* (rather than the dual) space X^* of a Banach space X.

From this point on we will always make the following assumption (unless explicitly stated otherwise):

Hypothesis 4.1. *Let $n \in \mathbb{N}$, $n \geq 2$, and assume that $\emptyset \neq \Omega \subset \mathbb{R}^n$ is a bounded Lipschitz domain.*

To discuss Sobolev spaces on the boundary of a Lipschitz domain, consider first the case where $\Omega \subset \mathbb{R}^n$ is the domain lying above the graph of a Lipschitz function $\varphi\colon \mathbb{R}^{n-1} \to \mathbb{R}$. In this setting, we define the Sobolev space $H^s(\partial\Omega)$ for $0 \le s \le 1$, as the space of functions $f \in L^2(\partial\Omega; d^{n-1}\omega)$ with the property that $f(x', \varphi(x'))$, as a function of $x' \in \mathbb{R}^{n-1}$, belongs to $H^s(\mathbb{R}^{n-1})$. This definition is easily adapted to the case when Ω is a Lipschitz domain whose boundary is compact, by using a smooth partition of unity. Finally, for $-1 \le s \le 0$, we set

$$H^s(\partial\Omega) = \big(H^{-s}(\partial\Omega)\big)^*, \quad -1 \leqslant s \leqslant 0. \tag{4.14}$$

From the above characterization of $H^s(\partial\Omega)$ it follows that any property of Sobolev spaces (of order $s \in [-1, 1]$) defined in Euclidean domains, which are invariant under multiplication by smooth, compactly supported functions as well as composition by bi-Lipschitz diffeomorphisms, readily extends to the setting of $H^s(\partial\Omega)$ (via localization and pullback). For additional background information in this context we refer, for instance, to [71, Chs. V, VI], [93, Ch. 1].

Assuming Hypothesis 4.1, we introduce the boundary trace operator γ_D^0 (the Dirichlet trace) by

$$\gamma_D^0\colon C(\overline{\Omega}) \to C(\partial\Omega), \quad \gamma_D^0 u = u|_{\partial\Omega}. \tag{4.15}$$

Then there exists a bounded, linear operator γ_D

$$\begin{aligned} &\gamma_D\colon H^s(\Omega) \to H^{s-(1/2)}(\partial\Omega) \hookrightarrow L^2(\partial\Omega; d^{n-1}\omega), \quad 1/2 < s < 3/2, \\ &\gamma_D\colon H^{3/2}(\Omega) \to H^{1-\varepsilon}(\partial\Omega) \hookrightarrow L^2(\partial\Omega; d^{n-1}\omega), \quad \varepsilon \in (0,1) \end{aligned} \tag{4.16}$$

(cf., e.g., [142, Theorem 3.38]), whose action is compatible with that of γ_D^0. That is, the two Dirichlet trace operators coincide on the intersection of their domains. Moreover, we recall that

$$\gamma_D\colon H^s(\Omega) \to H^{s-(1/2)}(\partial\Omega) \text{ is onto for } 1/2 < s < 3/2. \tag{4.17}$$

Next, retaining Hypothesis 4.1, we introduce the operator γ_N (the strong Neumann trace) by

$$\gamma_N = \nu \cdot \gamma_D \nabla\colon H^{s+1}(\Omega) \to L^2(\partial\Omega; d^{n-1}\omega), \quad 1/2 < s < 3/2, \tag{4.18}$$

where ν denotes the outward pointing normal unit vector to $\partial\Omega$. It follows from (4.16) that γ_N is also a bounded operator. We seek to extend the action of the Neumann trace operator (4.18) to other (related) settings. To set the stage, assume Hypothesis 4.1 and observe that the inclusion

$$\iota : H^{s_0}(\Omega) \hookrightarrow \big(H^r(\Omega)\big)^*, \quad s_0 > -1/2,\ r > 1/2, \tag{4.19}$$

is well defined and bounded. We then introduce the weak Neumann trace operator

$$\widetilde{\gamma}_N\colon \big\{u \in H^{s+1/2}(\Omega) \,\big|\, \Delta u \in H^{s_0}(\Omega)\big\} \to H^{s-1}(\partial\Omega), \quad s \in (0,1),\ s_0 > -1/2, \tag{4.20}$$

as follows: Given $u \in H^{s+1/2}(\Omega)$ with $\Delta u \in H^{s_0}(\Omega)$ for some $s \in (0,1)$ and $s_0 > -1/2$, we set (with ι as in (4.19) for $r := 3/2 - s > 1/2$)

$$\langle \phi, \widetilde{\gamma}_N u\rangle_{1-s} = {}_{H^{1/2-s}(\Omega)}\langle \nabla\Phi, \nabla u\rangle_{(H^{1/2-s}(\Omega))^*} + {}_{H^{3/2-s}(\Omega)}\langle \Phi, \iota(\Delta u)\rangle_{(H^{3/2-s}(\Omega))^*}, \tag{4.21}$$

for all $\phi \in H^{1-s}(\partial\Omega)$ and $\Phi \in H^{3/2-s}(\Omega)$ such that $\gamma_D\Phi = \phi$. We note that the first pairing in the right-hand side above is meaningful since

$$\big(H^{1/2-s}(\Omega)\big)^* = H^{s-1/2}(\Omega), \quad s \in (0,1), \tag{4.22}$$

that the definition (4.21) is independent of the particular extension Φ of ϕ, and that $\widetilde{\gamma}_N$ is a bounded extension of the Neumann trace operator γ_N defined in (4.18).

For further reference, let us also point out here that if $\Omega \subset \mathbb{R}^n$ is a bounded Lipschitz domain then for any $j,k \in \{1,\dots,n\}$ the (tangential first-order differential) operator

$$\partial/\partial\tau_{j,k} := \nu_j\partial_k - \nu_k\partial_j : H^s(\partial\Omega) \to H^{s-1}(\partial\Omega), \quad 0 \le s \le 1, \tag{4.23}$$

is well defined, linear and bounded. Assuming Hypothesis 4.1, we can then define the tangential gradient operator

$$\nabla_{tan} : \begin{cases} H^1(\partial\Omega) \to \big(L^2(\partial\Omega; d^{n-1}\omega)\big)^n \\ \qquad f \mapsto \nabla_{tan} f := \Big(\sum_{k=1}^n \nu_k \frac{\partial f}{\partial\tau_{kj}}\Big)_{1\le j\le n} \end{cases}, \quad f \in H^1(\partial\Omega). \tag{4.24}$$

The following result has been proved in [139].

Theorem 4.2. *Assume Hypothesis* 4.1 *and denote by* ν *the outward unit normal to* $\partial\Omega$. *Then the operator*

$$\gamma_2 : \begin{cases} H^2(\Omega) \to \big\{(g_0,g_1) \in H^1(\partial\Omega) \times L^2(\partial\Omega; d^{n-1}\omega) \,\big|\, \\ \qquad\qquad \nabla_{tan} g_0 + g_1\nu \in \big(H^{1/2}(\partial\Omega)\big)^n\big\} \\ \quad u \mapsto \gamma_2 u = (\gamma_D u\,,\, \gamma_N u), \end{cases} \tag{4.25}$$

is well defined, linear, bounded, onto, and has a linear, bounded right-inverse. The space $\big\{(g_0,g_1) \in H^1(\partial\Omega)\times L^2(\partial\Omega; d^{n-1}\omega) \,\big|\, \nabla_{tan}g_0 + g_1\nu \in \big(H^{1/2}(\partial\Omega)\big)^n\big\}$ *in* (4.25) *is equipped with the natural norm*

$$(g_0,g_1) \mapsto \|g_0\|_{H^1(\partial\Omega)} + \|g_1\|_{L^2(\partial\Omega;d^{n-1}\omega)} + \|\nabla_{tan}g_0 + g_1\nu\|_{(H^{1/2}(\partial\Omega))^n}. \tag{4.26}$$

Furthermore, the null space of the operator (4.25) *is given by*

$$\ker(\gamma_2) := \big\{u \in H^2(\Omega) \,\big|\, \gamma_D u = \gamma_N u = 0\big\} = H^2_0(\Omega), \tag{4.27}$$

with the latter space denoting the closure of $C_0^\infty(\Omega)$ *in* $H^2(\Omega)$.

Continuing to assume Hypothesis 4.1, we now introduce

$$N^{1/2}(\partial\Omega) := \big\{g \in L^2(\partial\Omega; d^{n-1}\omega) \,\big|\, g\nu_j \in H^{1/2}(\partial\Omega),\ 1 \le j \le n\big\}, \tag{4.28}$$

where the ν_j's are the components of ν. We equip this space with the natural norm

$$\|g\|_{N^{1/2}(\partial\Omega)} := \sum_{j=1}^{n} \|g\nu_j\|_{H^{1/2}(\partial\Omega)}. \tag{4.29}$$

Then $N^{1/2}(\partial\Omega)$ is a reflexive Banach space which embeds continuously into $L^2(\partial\Omega; d^{n-1}\omega)$. Furthermore,

$$N^{1/2}(\partial\Omega) = H^{1/2}(\partial\Omega) \text{ whenever } \Omega \text{ is a bounded } C^{1,r} \text{ domain with } r > 1/2. \tag{4.30}$$

It should be mentioned that the spaces $H^{1/2}(\partial\Omega)$ and $N^{1/2}(\partial\Omega)$ can be quite different for an arbitrary Lipschitz domain Ω. Our interest in the latter space stems from the fact that this arises naturally when considering the Neumann trace operator acting on

$$\big\{u \in H^2(\Omega) \,\big|\, \gamma_D u = 0\big\} = H^2(\Omega) \cap H^1_0(\Omega), \tag{4.31}$$

considered as a closed subspace of $H^2(\Omega)$ (hence, a Banach space when equipped with the H^2-norm). More specifically, we have (cf. [89] for a proof):

Lemma 4.3. *Assume Hypothesis* 4.1*. Then the Neumann trace operator* γ_N *considered in the context*

$$\gamma_N : H^2(\Omega) \cap H^1_0(\Omega) \to N^{1/2}(\partial\Omega) \tag{4.32}$$

is well defined, linear, bounded, onto and with a linear, bounded right-inverse. In addition, the null space of γ_N *in* (4.32) *is precisely* $H^2_0(\Omega)$*, the closure of* $C_0^\infty(\Omega)$ *in* $H^2(\Omega)$*.*

Most importantly for us here is the fact that one can use the above Neumann trace result in order to extend the action of the Dirichlet trace operator (4.16) to $\mathrm{dom}(-\Delta_{\max,\Omega})$, the domain of the maximal Laplacian, that is, $\{u \in L^2(\Omega; d^n x) \,|\, \Delta u \in L^2(\Omega; d^n x)\}$, which we consider equipped with the graph norm $u \mapsto \|u\|_{L^2(\Omega;d^n x)} + \|\Delta u\|_{L^2(\Omega;d^n x)}$. Specifically, with $\big(N^{1/2}(\partial\Omega)\big)^*$ denoting the conjugate dual space of $N^{1/2}(\partial\Omega)$, we have the following result from [89]:

Theorem 4.4. *Assume Hypothesis* 4.1*. Then there exists a unique linear, bounded operator*

$$\widehat{\gamma}_D : \big\{u \in L^2(\Omega; d^n x) \,\big|\, \Delta u \in L^2(\Omega; d^n x)\big\} \to \big(N^{1/2}(\partial\Omega)\big)^* \tag{4.33}$$

which is compatible with the Dirichlet trace introduced in (4.16)*, in the sense that, for each* $s > 1/2$*, one has*

$$\widehat{\gamma}_D u = \gamma_D u \text{ for every } u \in H^s(\Omega) \text{ with } \Delta u \in L^2(\Omega; d^n x). \tag{4.34}$$

Furthermore, this extension of the Dirichlet trace operator in (4.16) *allows for the following generalized integration by parts formula*

$${}_{N^{1/2}(\partial\Omega)}\langle \gamma_N w, \widehat{\gamma}_D u\rangle_{(N^{1/2}(\partial\Omega))^*} = (\Delta w, u)_{L^2(\Omega;d^n x)} - (w, \Delta u)_{L^2(\Omega;d^n x)}, \tag{4.35}$$

valid for every $u \in L^2(\Omega; d^n x)$ *with* $\Delta u \in L^2(\Omega; d^n x)$ *and every* $w \in H^2(\Omega) \cap H^1_0(\Omega)$*.*

We next review the case of the Neumann trace, whose action is extended to $\mathrm{dom}(-\Delta_{\max,\Omega})$. To this end, we need to address a number of preliminary matters. First, assuming Hypothesis 4.1, we make the following definition (compare with (4.28)):

$$N^{3/2}(\partial\Omega) := \big\{g \in H^1(\partial\Omega) \,\big|\, \nabla_{tan} g \in \big(H^{1/2}(\partial\Omega)\big)^n\big\}, \tag{4.36}$$

equipped with the natural norm

$$\|g\|_{N^{3/2}(\partial\Omega)} := \|g\|_{L^2(\partial\Omega;d^{n-1}\omega)} + \|\nabla_{tan} g\|_{(H^{1/2}(\partial\Omega))^n}. \tag{4.37}$$

Assuming Hypothesis 4.1, $N^{3/2}(\partial\Omega)$ is a reflexive Banach space which embeds continuously into the space $H^1(\partial\Omega; d^{n-1}\omega)$. In addition, this turns out to be a natural substitute for the more familiar space $H^{3/2}(\partial\Omega)$ in the case where Ω is sufficiently smooth. Concretely, one has

$$N^{3/2}(\partial\Omega) = H^{3/2}(\partial\Omega), \tag{4.38}$$

(as vector spaces with equivalent norms), whenever Ω is a bounded $C^{1,r}$ domain with $r > 1/2$. The primary reason we are interested in $N^{3/2}(\partial\Omega)$ is that this space arises naturally when considering the Dirichlet trace operator acting on

$$\big\{u \in H^2(\Omega) \,\big|\, \gamma_N u = 0\big\}, \tag{4.39}$$

considered as a closed subspace of $H^2(\Omega)$ (thus, a Banach space when equipped with the norm inherited from $H^2(\Omega)$). Concretely, the following result has been established in [89].

Lemma 4.5. *Assume Hypothesis* 4.1. *Then the Dirichlet trace operator γ_D considered in the context*

$$\gamma_D : \big\{u \in H^2(\Omega) \,\big|\, \gamma_N u = 0\big\} \to N^{3/2}(\partial\Omega) \tag{4.40}$$

is well defined, linear, bounded, onto and with a linear, bounded right-inverse. In addition, the null space of γ_D in (4.40) *is precisely $H_0^2(\Omega)$, the closure of $C_0^\infty(\Omega)$ in $H^2(\Omega)$.*

It is then possible to use the Neumann trace result from Lemma 4.5 in order to extend the action of the Neumann trace operator (4.18) to $\mathrm{dom}(-\Delta_{\max,\Omega}) = \big\{u \in L^2(\Omega; d^n x) \,\big|\, \Delta u \in L^2(\Omega; d^n x)\big\}$. As before, this space is equipped with the natural graph norm. Let $\big(N^{3/2}(\partial\Omega)\big)^*$ denote the conjugate dual space of $N^{3/2}(\partial\Omega)$. The following result holds:

Theorem 4.6. *Assume Hypothesis* 4.1. *Then there exists a unique linear, bounded operator*

$$\widehat{\gamma}_N : \big\{u \in L^2(\Omega; d^n x) \,\big|\, \Delta u \in L^2(\Omega; d^n x)\big\} \to \big(N^{3/2}(\partial\Omega)\big)^* \tag{4.41}$$

which is compatible with the Neumann trace introduced in (4.18)*, in the sense that, for each $s > 3/2$, one has*

$$\widehat{\gamma}_N u = \gamma_N u \ \text{ for every } u \in H^s(\Omega) \text{ with } \Delta u \in L^2(\Omega; d^n x). \tag{4.42}$$

Furthermore, this extension of the Neumann trace operator from (4.18) *allows for the following generalized integration by parts formula*

$$ {}_{N^{3/2}(\partial\Omega)}\langle \gamma_D w, \widehat{\gamma}_N u\rangle_{(N^{3/2}(\partial\Omega))^*} = (w, \Delta u)_{L^2(\Omega;d^nx)} - (\Delta w, u)_{L^2(\Omega;d^nx)}, \tag{4.43} $$

valid for every $u \in L^2(\Omega; d^nx)$ *with* $\Delta u \in L^2(\Omega; d^nx)$ *and every* $w \in H^2(\Omega)$ *with* $\gamma_N w = 0$.

A proof of Theorem 4.6 can be found in [89].

4.2. Perturbed Dirichlet and Neumann Laplacians

Here we shall discuss operators of the form $-\Delta + V$ equipped with Dirichlet and Neumann boundary conditions. Temporarily, we will employ the following assumptions:

Hypothesis 4.7. *Let* $n \in \mathbb{N}$, $n \geq 2$, *assume that* $\Omega \subset \mathbb{R}^n$ *is an open, bounded, nonempty set, and suppose that*

$$ V \in L^\infty(\Omega; d^nx) \ \text{ and } V \text{ is real valued a.e. on } \Omega. \tag{4.44} $$

We start by reviewing the perturbed Dirichlet and Neumann Laplacians $H_{D,\Omega}$ and $H_{N,\Omega}$ associated with an open set Ω in $\mathbb{R}^n$ and a potential V satisfying Hypothesis 4.7: Consider the sesquilinear forms in $L^2(\Omega; d^nx)$,

$$ Q_{D,\Omega}(u, v) = (\nabla u, \nabla v) + (u, Vv), \quad u, v \in \mathrm{dom}(Q_{D,\Omega}) = H_0^1(\Omega), \tag{4.45} $$

and

$$ Q_{N,\Omega}(u, v) = (\nabla u, \nabla v) + (u, Vv), \quad u, v \in \mathrm{dom}(Q_{N,\Omega}) = H^1(\Omega). \tag{4.46} $$

Then both forms in (4.45) and (4.46) are densely, defined, closed, and bounded from below in $L^2(\Omega; d^nx)$. Thus, by the first and second representation theorems for forms (cf., e.g., [114, Sect. VI.2]), one concludes that there exist unique self-adjoint operators $H_{D,\Omega}$ and $H_{N,\Omega}$ in $L^2(\Omega; d^nx)$, both bounded from below, associated with the forms $Q_{D,\Omega}$ and $Q_{N,\Omega}$, respectively, which satisfy

$$ Q_{D,\Omega}(u, v) = (u, H_{D,\Omega} v), \quad u \in \mathrm{dom}(Q_{D,\Omega}),\ v \in \mathrm{dom}(H_{D,\Omega}), \tag{4.47} $$

$$ \mathrm{dom}(H_{D,\Omega}) \subset \mathrm{dom}\left(|H_{D,\Omega}|^{1/2}\right) = \mathrm{dom}(Q_{D,\Omega}) = H_0^1(\Omega) \tag{4.48} $$

and

$$ Q_{N,\Omega}(u, v) = (u, H_{N,\Omega} v), \quad u \in \mathrm{dom}(Q_{N,\Omega}),\ v \in \mathrm{dom}(H_{N,\Omega}), \tag{4.49} $$

$$ \mathrm{dom}(H_{N,\Omega}) \subset \mathrm{dom}\left(|H_{N,\Omega}|^{1/2}\right) = \mathrm{dom}(Q_{N,\Omega}) = H^1(\Omega). \tag{4.50} $$

In the case of the perturbed Dirichlet Laplacian, $H_{D,\Omega}$, one actually can say a bit more: Indeed, $H_{D,\Omega}$ coincides with the Friedrichs extension of the operator

$$ H_{c,\Omega} u = (-\Delta + V)u, \quad u \in \mathrm{dom}(H_{c,\Omega}) := C_0^\infty(\Omega) \tag{4.51} $$

in $L^2(\Omega; d^nx)$,

$$ (H_{c,\Omega})_F = H_{D,\Omega}, \tag{4.52} $$

and one obtains as an immediate consequence of (2.19) and (4.45)

$$H_{D,\Omega}u = (-\Delta + V)u, \quad u \in \operatorname{dom}(H_{D,\Omega}) = \big\{v \in H_0^1(\Omega) \,\big|\, \Delta v \in L^2(\Omega; d^n x)\big\}. \tag{4.53}$$

(We also refer to [71, Sect. IV.2, Theorem VII.1.4].) In addition, $H_{D,\Omega}$ is known to have a compact resolvent and hence purely discrete spectrum bounded from below.

In the case of the perturbed Neumann Laplacian, $H_{N,\Omega}$, it is not possible to be more specific under this general hypothesis on Ω just being open. However, under the additional assumptions on the domain Ω in Hypothesis 4.1 one can be more explicit about the domain of $H_{N,\Omega}$ and also characterize its spectrum as follows. In addition, we also record an improvement of (4.53) under the additional Lipschitz hypothesis on Ω:

Theorem 4.8. *Assume Hypotheses* 4.1 *and* 4.7*. Then the perturbed Dirichlet Laplacian, $H_{D,\Omega}$, given by*

$$\begin{aligned} &H_{D,\Omega}u = (-\Delta + V)u, \\ &u \in \operatorname{dom}(H_{D,\Omega}) = \big\{v \in H^1(\Omega) \,\big|\, \Delta v \in L^2(\Omega; d^n x),\, \gamma_D v = 0 \text{ in } H^{1/2}(\partial\Omega)\big\} \\ &\qquad\qquad\qquad\; = \big\{v \in H_0^1(\Omega) \,\big|\, \Delta v \in L^2(\Omega; d^n x)\big\}, \end{aligned} \tag{4.54}$$

is self-adjoint and bounded from below in $L^2(\Omega; d^n x)$. Moreover,

$$\operatorname{dom}\big(|H_{D,\Omega}|^{1/2}\big) = H_0^1(\Omega), \tag{4.55}$$

and the spectrum of $H_{D,\Omega}$, is purely discrete (i.e., it consists of eigenvalues of finite multiplicity),

$$\sigma_{\rm ess}(H_{D,\Omega}) = \emptyset. \tag{4.56}$$

If, in addition, $V \geq 0$ a.e. in Ω, then $H_{D,\Omega}$ is strictly positive in $L^2(\Omega; d^n x)$.

The corresponding result for the perturbed Neumann Laplacian $H_{N,\Omega}$ reads as follows:

Theorem 4.9. *Assume Hypotheses* 4.1 *and* 4.7*. Then the perturbed Neumann Laplacian, $H_{N,\Omega}$, given by*

$$\begin{aligned} &H_{N,\Omega}u = (-\Delta + V)u, \\ &u \in \operatorname{dom}(H_{N,\Omega}) = \big\{v \in H^1(\Omega) \,\big|\, \Delta v \in L^2(\Omega; d^n x),\, \widetilde\gamma_N v = 0 \text{ in } H^{-1/2}(\partial\Omega)\big\}, \end{aligned} \tag{4.57}$$

is self-adjoint and bounded from below in $L^2(\Omega; d^n x)$. Moreover,

$$\operatorname{dom}\big(|H_{N,\Omega}|^{1/2}\big) = H^1(\Omega), \tag{4.58}$$

and the spectrum of $H_{N,\Omega}$, is purely discrete (i.e., it consists of eigenvalues of finite multiplicity),

$$\sigma_{\rm ess}(H_{N,\Omega}) = \emptyset. \tag{4.59}$$

If, in addition, $V \geq 0$ a.e. in Ω, then $H_{N,\Omega}$ is nonnegative in $L^2(\Omega; d^n x)$.

In the sequel, corresponding to the case where $V \equiv 0$, we shall abbreviate

$$-\Delta_{D,\Omega} \text{ and } -\Delta_{N,\Omega}, \tag{4.60}$$

for $H_{D,\Omega}$ and $H_{N,\Omega}$, respectively, and simply refer to these operators as, the Dirichlet and Neumann Laplacians. The above results have been proved in [84, App. A], [90] for considerably more general potentials than assumed in Hypothesis 4.7.

Next, we shall now consider the minimal and maximal perturbed Laplacians. Concretely, given an open set $\Omega \subset \mathbb{R}^n$ and a potential $0 \leq V \in L^\infty(\Omega; d^n x)$, we introduce the maximal perturbed Laplacian in $L^2(\Omega; d^n x)$

$$\begin{aligned} &H_{\max,\Omega} u := (-\Delta + V)u, \\ &u \in \operatorname{dom}(H_{\max,\Omega}) := \big\{v \in L^2(\Omega; d^n x) \,\big|\, \Delta v \in L^2(\Omega; d^n x)\big\}. \end{aligned} \tag{4.61}$$

We pause for a moment to dwell on the notation used in connection with the symbol Δ:

Remark 4.10. Throughout this manuscript the symbol Δ alone indicates that the Laplacian acts in the sense of distributions,

$$\Delta \colon \mathcal{D}'(\Omega) \to \mathcal{D}'(\Omega). \tag{4.62}$$

In some cases, when it is necessary to interpret Δ as a bounded operator acting between Sobolev spaces, we write $\Delta \in \mathcal{B}\big(H^s(\Omega), H^{s-2}(\Omega)\big)$ for various ranges of $s \in \mathbb{R}$ (which is of course compatible with (4.62)). In addition, as a consequence of standard interior elliptic regularity (cf. Weyl's classical lemma) it is not difficult to see that if $\Omega \subseteq \mathbb{R}$ is open, $u \in \mathcal{D}'(\Omega)$ and $\Delta u \in L^2_{\text{loc}}(\Omega; d^n x)$ then actually $u \in H^2_{\text{loc}}(\Omega)$. In particular, this comment applies to $u \in \operatorname{dom}(H_{\max,\Omega})$ in (4.61).

In the remainder of this subsection we shall collect a number of results, originally proved in [89] when $V \equiv 0$, but which are easily seen to hold in the more general setting considered here.

Lemma 4.11. *Assume Hypotheses* 4.1 *and* 4.7*. Then the maximal perturbed Laplacian associated with* Ω *and the potential* V *is a closed, densely defined operator for which*

$$\begin{aligned} H^2_0(\Omega) &\subseteq \operatorname{dom}((H_{\max,\Omega})^*) \\ &\subseteq \big\{u \in L^2(\Omega; d^n x) \,\big|\, \Delta u \in L^2(\Omega; d^n x),\, \widehat{\gamma}_D u = \widehat{\gamma}_N u = 0\big\}. \end{aligned} \tag{4.63}$$

For an open set $\Omega \subset \mathbb{R}^n$ and a potential $0 \leq V \in L^\infty(\Omega; d^n x)$, we also bring in the minimal perturbed Laplacian in $L^2(\Omega; d^n x)$, that is,

$$H_{\min,\Omega} u := (-\Delta + V)u, \quad u \in \operatorname{dom}(H_{\min,\Omega}) := H^2_0(\Omega). \tag{4.64}$$

Corollary 4.12. *Assume Hypotheses* 4.1 *and* 4.7*. Then* $H_{\min,\Omega}$ *is a densely defined, symmetric operator which satisfies*

$$H_{\min,\Omega} \subseteq (H_{\max,\Omega})^* \text{ and } H_{\max,\Omega} \subseteq (H_{\min,\Omega})^*. \tag{4.65}$$

Equality occurs in one (*and hence, both*) *inclusions in* (4.65) *if and only if*

$$H^2_0(\Omega) \text{ equals } \big\{u \in L^2(\Omega; d^n x) \,\big|\, \Delta u \in L^2(\Omega; d^n x),\, \widehat{\gamma}_D u = \widehat{\gamma}_N u = 0\big\}. \tag{4.66}$$

5. Boundary value problems in quasi-convex domains

This section is divided into three parts. In Subsection 5.1 we introduce a distinguished category of the family of Lipschitz domains in $\mathbb{R}^n$, called quasi-convex domains, which is particularly well suited for the kind of analysis we have in mind. In Subsection 5.2 and Subsection 5.3, we then proceed to review, respectively, trace operators and boundary problems, and Dirichlet-to-Neumann operators in quasi-convex domains.

5.1. The class of quasi-convex domains

In the class of Lipschitz domains, the two spaces appearing in (4.66) are not necessarily equal (although, obviously, the left-to-right inclusion always holds). The question now arises: What extra properties of the Lipschitz domain will guarantee equality in (4.66)? This issue has been addressed in [89], where a class of domains (which is in the nature of best possible) has been identified.

To describe this class, we need some preparations. Given $n \geq 1$, denote by $MH^{1/2}(\mathbb{R}^n)$ the class of pointwise multipliers of the Sobolev space $H^{1/2}(\mathbb{R}^n)$. That is,

$$MH^{1/2}(\mathbb{R}^n) := \big\{f \in L^1_{\rm loc}(\mathbb{R}^n) \,\big|\, M_f \in \mathcal{B}\big(H^{1/2}(\mathbb{R}^n)\big)\big\}, \tag{5.1}$$

where M_f is the operator of pointwise multiplication by f. This space is equipped with the natural norm, that is,

$$\|f\|_{MH^{1/2}(\mathbb{R}^n)} := \|M_f\|_{\mathcal{B}(H^{1/2}(\mathbb{R}^n))}. \tag{5.2}$$

For a comprehensive and systematic treatment of spaces of multipliers, the reader is referred to the 1985 monograph of Maz'ya and Shaposhnikova [140]. Following [140], [141], we now introduce a special class of domains, whose boundary regularity properties are expressed in terms of spaces of multipliers.

Definition 5.1. Given $\delta > 0$, call a bounded, Lipschitz domain $\Omega \subset \mathbb{R}^n$ to be of class $MH^{1/2}_\delta$, and write

$$\partial\Omega \in MH^{1/2}_\delta, \tag{5.3}$$

provided the following holds: There exists a finite open covering $\{\mathcal{O}_j\}_{1\leq j\leq N}$ of the boundary $\partial\Omega$ of Ω such that for every $j \in \{1,\dots,N\}$, $\mathcal{O}_j \cap \Omega$ coincides with the portion of $\mathcal{O}_j$ lying in the over-graph of a Lipschitz function $\varphi_j : \mathbb{R}^{n-1} \to \mathbb{R}$ (considered in a new system of coordinates obtained from the original one via a rigid motion) which, additionally, has the property that

$$\nabla\varphi_j \in \big(MH^{1/2}(\mathbb{R}^{n-1})\big)^n \ \text{ and } \ \|\varphi_j\|_{(MH^{1/2}(\mathbb{R}^{n-1}))^n} \leq \delta. \tag{5.4}$$

Going further, we consider the classes of domains

$$MH^{1/2}_\infty := \bigcup_{\delta>0} MH^{1/2}_\delta, \quad MH^{1/2}_0 := \bigcap_{\delta>0} MH^{1/2}_\delta, \tag{5.5}$$

and also introduce the following definition:

Definition 5.2. We call a bounded Lipschitz domain $\Omega \subset \mathbb{R}^n$ to be *square-Dini*, and write

$$\partial\Omega \in \mathrm{SD}, \tag{5.6}$$

provided the following holds: There exists a finite open covering $\{\mathcal{O}_j\}_{1\le j\le N}$ of the boundary $\partial\Omega$ of Ω such that for every $j \in \{1,\dots,N\}$, $\mathcal{O}_j \cap \Omega$ coincides with the portion of $\mathcal{O}_j$ lying in the over-graph of a Lipschitz function $\varphi_j : \mathbb{R}^{n-1} \to \mathbb{R}$ (considered in a new system of coordinates obtained from the original one via a rigid motion) which, additionally, has the property that the following square-Dini condition holds,

$$\int_0^1 \frac{dt}{t}\left(\frac{\omega(\nabla\varphi_j;t)}{t^{1/2}}\right)^2 < \infty. \tag{5.7}$$

Here, given a (possibly vector-valued) function f in $\mathbb{R}^{n-1}$,

$$\omega(f;t) := \sup\{|f(x)-f(y)|\,|\,x,y\in\mathbb{R}^{n-1},\ |x-y|\le t\}, \quad t\in(0,1), \tag{5.8}$$

is the modulus of continuity of f, at scale t.

From the work of Maz'ya and Shaposhnikova [140] [141], it is known that if $r > 1/2$, then

$$\Omega \in C^{1,r} \Longrightarrow \Omega \in \mathrm{SD} \Longrightarrow \Omega \in MH_0^{1/2} \Longrightarrow \Omega \in MH_\infty^{1/2}. \tag{5.9}$$

As pointed out in [141], domains of class $MH_\infty^{1/2}$ can have certain types of vertices and edges when $n \ge 3$. Thus, the domains in this class can be nonsmooth.

Next, we recall that a domain is said to satisfy a uniform exterior ball condition (UEBC) provided there exists a number $r > 0$ with the property that

$$\begin{aligned} &\text{for every } x\in\partial\Omega, \text{ there exists } y\in\mathbb{R}^n, \text{ such that } B(y,r)\cap\Omega=\emptyset \\ &\quad \text{and } x\in\partial B(y,r)\cap\partial\Omega. \end{aligned} \tag{5.10}$$

Heuristically, (5.10) should be interpreted as a lower bound on the curvature of $\partial\Omega$. Next, we review the class of almost-convex domains introduced in [146].

Definition 5.3. A bounded Lipschitz domain $\Omega \subset \mathbb{R}^n$ is called an almost-convex domain provided there exists a family $\{\Omega_\ell\}_{\ell\in\mathbb{N}}$ of open sets in $\mathbb{R}^n$ with the following properties:

(i) $\partial\Omega_\ell \in C^2$ and $\overline{\Omega_\ell} \subset \Omega$ for every $\ell \in \mathbb{N}$.

(ii) $\Omega_\ell \nearrow \Omega$ as $\ell \to \infty$, in the sense that $\overline{\Omega_\ell} \subset \Omega_{\ell+1}$ for each $\ell \in \mathbb{N}$ and $\bigcup_{\ell\in\mathbb{N}} \Omega_\ell = \Omega$.

(iii) There exists a neighborhood U of $\partial\Omega$ and, for each $\ell \in \mathbb{N}$, a C^2 real-valued function ρ_ℓ defined in U with the property that $\rho_\ell < 0$ on $U \cap \Omega_\ell$, $\rho_\ell > 0$ in $U\backslash\overline{\Omega_\ell}$, and ρ_ℓ vanishes on $\partial\Omega_\ell$. In addition, it is assumed that there exists some constant $C_1 \in (1,\infty)$ such that

$$C_1^{-1} \le |\nabla\rho_\ell(x)| \le C_1, \quad x\in\partial\Omega_\ell,\ \ell\in\mathbb{N}. \tag{5.11}$$

(iv) There exists $C_2 \geq 0$ such that for every number $\ell \in \mathbb{N}$, every point $x \in \partial\Omega_\ell$, and every vector $\xi \in \mathbb{R}^n$ which is tangent to $\partial\Omega_\ell$ at x, there holds

$$\big\langle \mathrm{Hess}\,(\rho_\ell)\xi\,,\,\xi\big\rangle \geq -C_2|\xi|^2, \tag{5.12}$$

where $\langle\,\cdot\,,\,\cdot\,\rangle$ is the standard Euclidean inner product in $\mathbb{R}^n$ and

$$\mathrm{Hess}\,(\rho_\ell) := \left(\frac{\partial^2\rho_\ell}{\partial x_j\partial x_k}\right)_{1\leq j,k\leq n}, \tag{5.13}$$

is the Hessian of ρ_ℓ.

A few remarks are in order: First, it is not difficult to see that (5.11) ensures that each domain Ω_ℓ is Lipschitz, with Lipschitz constant bounded uniformly in ℓ. Second, (5.12) simply says that, as quadratic forms on the tangent bundle $T\partial\Omega_\ell$ to $\partial\Omega_\ell$, one has

$$\mathrm{Hess}\,(\rho_\ell) \geq -C_2\, I_n, \tag{5.14}$$

where I_n is the $n\times n$ identity matrix. Hence, another equivalent formulation of (5.12) is the following requirement:

$$\sum_{j,k=1}^{n}\frac{\partial^2\rho_\ell}{\partial x_j\partial x_k}\xi_j\xi_k \geq -C_2\sum_{j=1}^{n}\xi_j^2, \ \text{ whenever } \ \rho_\ell = 0 \ \text{ and } \ \sum_{j=1}^{n}\frac{\partial\rho_\ell}{\partial x_j}\xi_j = 0. \tag{5.15}$$

We note that, since the second fundamental form II_ℓ on $\partial\Omega_\ell$ is $II_\ell = \mathrm{Hess}\,\rho_\ell/|\nabla\rho_\ell|$, almost-convexity is, in view of (5.11), equivalent to requiring that II_ℓ be bounded from below, uniformly in ℓ.

We now discuss some important special classes of almost-convex domains.

Definition 5.4. A bounded Lipschitz domain $\Omega\subset\mathbb{R}^n$ satisfies a local exterior ball condition, henceforth referred to as LEBC, if every boundary point $x_0\in\partial\Omega$ has an open neighborhood $\mathcal{O}$ which satisfies the following two conditions:

(i) There exists a Lipschitz function $\varphi:\mathbb{R}^{n-1}\to\mathbb{R}$ with $\varphi(0)=0$ such that if D is the domain above the graph of φ, then D satisfies a UEBC.

(ii) There exists a $C^{1,1}$ diffeomorphism Υ mapping $\mathcal{O}$ onto the unit ball $B(0,1)$ in $\mathbb{R}^n$ such that $\Upsilon(x_0)=0$, $\Upsilon(\mathcal{O}\cap\Omega)=B(0,1)\cap D$, $\Upsilon(\mathcal{O}\backslash\overline{\Omega})=B(0,1)\backslash\overline{D}$.

It is clear from Definition 5.4 that the class of bounded domains satisfying a LEBC is invariant under $C^{1,1}$ diffeomorphisms. This makes this class of domains amenable to working on manifolds. This is the point of view adopted in [146], where the following result is also proved:

Lemma 5.5. *If the bounded Lipschitz domain $\Omega\subset\mathbb{R}^n$ satisfies a LEBC then it is almost-convex.*

Hence, in the class of bounded Lipschitz domains in $\mathbb{R}^n$, we have

$$\text{convex} \Longrightarrow \text{UEBC} \Longrightarrow \text{LEBC} \Longrightarrow \text{almost-convex}. \tag{5.16}$$

We are now in a position to specify the class of domains in which most of our subsequent analysis will be carried out.

Definition 5.6. Let $n \in \mathbb{N}$, $n \geq 2$, and assume that $\Omega \subset \mathbb{R}^n$ is a bounded Lipschitz domain. Then Ω is called a quasi-convex domain if there exists $\delta > 0$ sufficiently small (relative to n and the Lipschitz character of Ω), with the following property that for every $x \in \partial\Omega$ there exists an open subset Ω_x of Ω such that $\partial\Omega \cap \partial\Omega_x$ is an open neighborhood of x in $\partial\Omega$, and for which one of the following two conditions holds:

(i) Ω_x is of class $MH^{1/2}_\delta$ if $n \geq 3$, and of class $C^{1,r}$ for some $1/2 < r < 1$ if $n = 2$.

(ii) Ω_x is an almost-convex domain.

Given Definition 5.6, we thus introduce the following basic assumption:

Hypothesis 5.7. *Let $n \in \mathbb{N}$, $n \geq 2$, and assume that $\Omega \subset \mathbb{R}^n$ is a quasi-convex domain.*

Informally speaking, the above definition ensures that the boundary singularities are directed outwardly. A typical example of such a domain is shown in Figure 1 below.

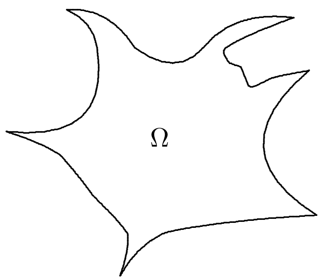

FIGURE 1. A quasi-convex domain.

Being quasi-convex is a certain type of regularity condition of the boundary of a Lipschitz domain. The only way we are going to utilize this property is via the following elliptic regularity result proved in [89].

Proposition 5.8. *Assume Hypotheses* 4.7 *and* 5.7*. Then*

$$\operatorname{dom}\big(H_{D,\Omega}\big) \subset H^2(\Omega), \quad \operatorname{dom}\big(H_{N,\Omega}\big) \subset H^2(\Omega). \tag{5.17}$$

In fact, all of our results in this survey hold in the class of Lipschitz domains for which the two inclusions in (5.17) hold.

The following theorem addresses the issue raised at the beginning of this subsection. Its proof is similar to the special case $V \equiv 0$, treated in [89].

Theorem 5.9. *Assume Hypotheses* 4.7 *and* 5.7*. Then* (4.66) *holds. In particular,*

$$\begin{aligned} \operatorname{dom}(H_{\min,\Omega}) &= H^2_0(\Omega) \\ &= \big\{u \in L^2(\Omega; d^n x) \,\big|\, \Delta u \in L^2(\Omega; d^n x),\, \widehat{\gamma}_D u = \widehat{\gamma}_N u = 0\big\}, \end{aligned} \tag{5.18}$$

$$\operatorname{dom}(H_{\max,\Omega}) = \big\{u \in L^2(\Omega; d^n x) \,\big|\, \Delta u \in L^2(\Omega; d^n x)\big\}, \tag{5.19}$$

and

$$H_{\min,\Omega} = (H_{\max,\Omega})^* \ \ and \ \ H_{\max,\Omega} = (H_{\min,\Omega})^*. \tag{5.20}$$

We conclude this subsection with the following result which is essentially contained in [89].

Proposition 5.10. *Assume Hypotheses* 4.1 *and* 4.7*. Then the Friedrichs extension of* $(-\Delta + V)|_{C_0^\infty(\Omega)}$ *in* $L^2(\Omega; d^n x)$ *is precisely the perturbed Dirichlet Laplacian* $H_{D,\Omega}$*. Consequently, if Hypothesis* 5.7 *is assumed in place of Hypothesis* 4.1*, then the Friedrichs extension of* $H_{\min,\Omega}$ *in* (4.64) *is the perturbed Dirichlet Laplacian* $H_{D,\Omega}$*.*

5.2. Trace operators and boundary problems on quasi-convex domains

Here we revisit the issue of traces, originally taken up in Section 2, and extend the scope of this theory. The goal is to extend our earlier results to a context that is well suited for the treatment of the perturbed Krein Laplacian in quasi-convex domains, later on. All results in this subsection are direct generalizations of similar results proved in the case where $V \equiv 0$ in [89].

Theorem 5.11. *Assume Hypotheses* 4.7 *and* 5.7*, and suppose that* $z \in \mathbb{C}\backslash\sigma(H_{D,\Omega})$*. Then for any functions* $f \in L^2(\Omega; d^n x)$ *and* $g \in (N^{1/2}(\partial\Omega))^*$ *the following inhomogeneous Dirichlet boundary value problem*

$$\begin{cases} (-\Delta + V - z)u = f \ \text{ in } \ \Omega, \\ u \in L^2(\Omega; d^n x), \\ \widehat{\gamma}_D u = g \ \text{ on } \ \partial\Omega, \end{cases} \tag{5.21}$$

has a unique solution $u = u_D$*. This solution satisfies*

$$\|u_D\|_{L^2(\Omega;d^n x)} + \|\widehat{\gamma}_N u_D\|_{(N^{3/2}(\partial\Omega))^*} \leq C_D(\|f\|_{L^2(\Omega;d^n x)} + \|g\|_{(N^{1/2}(\partial\Omega))^*}) \tag{5.22}$$

for some constant $C_D = C_D(\Omega, V, z) > 0$*, and the following regularity results hold:*

$$g \in H^1(\partial\Omega) \ \text{ implies } \ u_D \in H^{3/2}(\Omega), \tag{5.23}$$

$$g \in \gamma_D\big(H^2(\Omega)\big) \ \text{ implies } \ u_D \in H^2(\Omega). \tag{5.24}$$

In particular,

$$g = 0 \ \text{ implies } \ u_D \in H^2(\Omega) \cap H_0^1(\Omega). \tag{5.25}$$

Natural estimates are valid in each case.

Moreover, the solution operator for (5.21) *with* $f = 0$ *(i.e.,* $P_{D,\Omega,V,z} : g \mapsto u_D$*) satisfies*

$$P_{D,\Omega,V,z} = \big[\gamma_N(H_{D,\Omega} - \overline{z}I_\Omega)^{-1}\big]^* \in \mathcal{B}\big((N^{1/2}(\partial\Omega))^*, L^2(\Omega; d^n x)\big), \tag{5.26}$$

and the solution of (5.21) *is given by the formula*

$$u_D = (H_{D,\Omega} - zI_\Omega)^{-1} f - \big[\gamma_N(H_{D,\Omega} - \overline{z}I_\Omega)^{-1}\big]^* g. \tag{5.27}$$

Corollary 5.12. *Assume Hypotheses* 4.7 *and* 5.7*. Then for every* $z \in \mathbb{C}\backslash\sigma(H_{D,\Omega})$ *the map*

$$\widehat{\gamma}_D : \big\{u \in L^2(\Omega; d^n x) \,\big|\, (-\Delta + V - z)u = 0 \, in\, \Omega\big\} \to \big(N^{1/2}(\partial\Omega)\big)^* \tag{5.28}$$

is an isomorphism (*i.e., bijective and bicontinuous*)*.*

Theorem 5.13. *Assume Hypotheses* 4.7 *and* 5.7 *and suppose that* $z \in \mathbb{C}\backslash\sigma(H_{N,\Omega})$*. Then for any functions* $f \in L^2(\Omega; d^n x)$ *and* $g \in (N^{3/2}(\partial\Omega))^*$ *the following inhomogeneous Neumann boundary value problem*

$$\begin{cases} (-\Delta + V - z)u = f \;\; in \;\; \Omega, \\ u \in L^2(\Omega; d^n x), \\ \widehat{\gamma}_N u = g \;\; on \;\; \partial\Omega, \end{cases} \tag{5.29}$$

has a unique solution $u = u_N$*. This solution satisfies*

$$\|u_N\|_{L^2(\Omega;d^n x)} + \|\widehat{\gamma}_D u_N\|_{(N^{1/2}(\partial\Omega))^*} \leq C_N (\|f\|_{L^2(\Omega;d^n x)} + \|g\|_{(N^{3/2}(\partial\Omega))^*}) \tag{5.30}$$

for some constant $C_N = C_N(\Omega, V, z) > 0$*, and the following regularity results hold:*

$$g \in L^2(\partial\Omega; d^{n-1}\omega) \;\; implies \;\; u_N \in H^{3/2}(\Omega), \tag{5.31}$$

$$g \in \gamma_N\big(H^2(\Omega)\big) \;\; implies \;\; u_N \in H^2(\Omega). \tag{5.32}$$

Natural estimates are valid in each case.

Moreover, the solution operator for (5.29) *with* $f = 0$ (*i.e.,* $P_{N,\Omega,V,z} : g \mapsto u_N$) *satisfies*

$$P_{N,\Omega,V,z} = \big[\gamma_D (H_{N,\Omega} - \overline{z} I_\Omega)^{-1}\big]^* \in \mathcal{B}\big((N^{3/2}(\partial\Omega))^*, L^2(\Omega; d^n x)\big), \tag{5.33}$$

and the solution of (5.29) *is given by the formula*

$$u_N = (H_{N,\Omega} - z I_\Omega)^{-1} f + \big[\gamma_D (H_{N,\Omega} - \overline{z} I_\Omega)^{-1}\big]^* g. \tag{5.34}$$

Corollary 5.14. *Assume Hypotheses* 4.7 *and* 5.7*. Then, for every* $z \in \mathbb{C}\backslash\sigma(H_{N,\Omega})$*, the map*

$$\widehat{\gamma}_N : \big\{u \in L^2(\Omega; d^n x) \,\big|\, (-\Delta + V - z)u = 0 \;\; in \; \Omega\big\} \to \big(N^{3/2}(\partial\Omega)\big)^* \tag{5.35}$$

is an isomorphism (*i.e., bijective and bicontinuous*)*.*

5.3. Dirichlet-to-Neumann operators on quasi-convex domains

In this subsection we review spectral parameter-dependent Dirichlet-to-Neumann maps, also known in the literature as Weyl–Titchmarsh and Poincaré–Steklov operators. Assuming Hypotheses 4.7 and 5.7, introduce the Dirichlet-to-Neumann map $M_{D,N,\Omega,V}(z)$ associated with $-\Delta + V - z$ on Ω, as follows:

$$M_{D,N,\Omega,V}(z)\colon \begin{cases} \big(N^{1/2}(\partial\Omega)\big)^* \to \big(N^{3/2}(\partial\Omega)\big)^*, \\ \qquad\qquad f \mapsto -\widehat{\gamma}_N u_D, \end{cases} \quad z \in \mathbb{C}\backslash\sigma(H_{D,\Omega}), \tag{5.36}$$

where u_D is the unique solution of

$$(-\Delta + V - z)u = 0 \;\text{ in } \Omega, \quad u \in L^2(\Omega; d^n x), \;\; \widehat{\gamma}_D u = f \;\text{ on } \partial\Omega. \tag{5.37}$$

Retaining Hypotheses 4.7 and 5.7, we next introduce the Neumann-to-Dirichlet map $M_{N,D,\Omega,V}(z)$ associated with $-\Delta + V - z$ on Ω, as follows:

$$M_{N,D,\Omega,V}(z)\colon \begin{cases} \big(N^{3/2}(\partial\Omega)\big)^* \to \big(N^{1/2}(\partial\Omega)\big)^*, \\ \qquad\qquad g \mapsto \widehat{\gamma}_D u_N, \end{cases} \quad z\in\mathbb{C}\backslash\sigma(H_{N,\Omega}), \tag{5.38}$$

where u_N is the unique solution of

$$(-\Delta + V - z)u = 0 \text{ in } \Omega, \quad u\in L^2(\Omega;d^nx), \;\; \widehat{\gamma}_N u = g \text{ on } \partial\Omega. \tag{5.39}$$

As in [89], where the case $V\equiv 0$ has been treated, we then have the following result:

Theorem 5.15. *Assume Hypotheses* 4.7 *and* 5.7. *Then, with the above notation,*

$$M_{D,N,\Omega,V}(z)\in\mathcal{B}\big((N^{1/2}(\partial\Omega))^*\,,\,(N^{3/2}(\partial\Omega))^*\big), \quad z\in\mathbb{C}\backslash\sigma(H_{D,\Omega}), \tag{5.40}$$

and

$$M_{D,N,\Omega,V}(z) = \widehat{\gamma}_N\big[\gamma_N(H_{D,\Omega}-\overline{z}I_\Omega)^{-1}\big]^*, \quad z\in\mathbb{C}\backslash\sigma(H_{D,\Omega}). \tag{5.41}$$

Similarly,

$$M_{N,D,\Omega,V}(z)\in\mathcal{B}\big((N^{3/2}(\partial\Omega))^*\,,\,(N^{1/2}(\partial\Omega))^*\big), \quad z\in\mathbb{C}\backslash\sigma(H_{N,\Omega}), \tag{5.42}$$

and

$$M_{N,D,\Omega,V}(z) = \widehat{\gamma}_D\big[\gamma_D(H_{N,\Omega}-\overline{z}I_\Omega)^{-1}\big]^*, \quad z\in\mathbb{C}\backslash\sigma(H_{N,\Omega}). \tag{5.43}$$

Moreover,

$$M_{N,D,\Omega,V}(z) = -M_{D,N,\Omega,V}(z)^{-1}, \quad z\in\mathbb{C}\backslash(\sigma(H_{D,\Omega})\cup\sigma(H_{N,\Omega})), \tag{5.44}$$

and

$$\big[M_{D,N,\Omega,V}(z)\big]^* = M_{D,N,\Omega,V}(\overline{z}), \quad \big[M_{N,D,\Omega,V}(z)\big]^* = M_{N,D,\Omega,V}(\overline{z}). \tag{5.45}$$

As a consequence, one also has

$$M_{D,N,\Omega,V}(z)\in\mathcal{B}\big(N^{3/2}(\partial\Omega)\,,\,N^{1/2}(\partial\Omega)\big), \quad z\in\mathbb{C}\backslash\sigma(H_{D,\Omega}), \tag{5.46}$$

$$M_{N,D,\Omega,V}(z)\in\mathcal{B}\big(N^{1/2}(\partial\Omega)\,,\,N^{3/2}(\partial\Omega)\big), \quad z\in\mathbb{C}\backslash\sigma(H_{N,\Omega}). \tag{5.47}$$

For closely related recent work on Weyl–Titchmarsh operators associated with nonsmooth domains we refer to [86], [87], [88], [89], and [90]. For an extensive list of references on z-dependent Dirichlet-to-Neumann maps we also refer, for instance, to [7], [11], [15], [35], [48], [50], [51], [52], [53], [65], [66], [84]–[90], [99], [101], [158], [164], [165], [166].

6. Regularized Neumann traces and perturbed Krein Laplacians

This section is structured into two parts dealing, respectively, with the regularized Neumann trace operator (Subsection 6.1), and the perturbed Krein Laplacian in quasi-convex domains (Subsection 6.2).

6.1. The regularized Neumann trace operator on quasi-convex domains

Following earlier work in [89], we now consider a version of the Neumann trace operator which is suitably normalized to permit the familiar version of Green's formula (cf. (6.8) below) to work in the context in which the functions involved are only known to belong to $\operatorname{dom}(-\Delta_{\max,\Omega})$. The following theorem is a slight extension of a similar result proved in [89] when $V \equiv 0$.

Theorem 6.1. *Assume Hypotheses* 4.7 *and* 5.7. *Then, for every* $z \in \mathbb{C}\backslash\sigma(H_{D,\Omega})$, *the map*

$$\tau_{N,V,z} : \big\{u \in L^2(\Omega; d^n x);\ \Delta u \in L^2(\Omega; d^n x)\big\} \to N^{1/2}(\partial\Omega) \tag{6.1}$$

given by

$$\tau_{N,V,z} u := \widehat{\gamma}_N u + M_{D,N,\Omega,V}(z)\big(\widehat{\gamma}_D u\big), \quad u \in L^2(\Omega; d^n x),\ \Delta u \in L^2(\Omega; d^n x), \tag{6.2}$$

is well defined, linear and bounded, where the space

$$\big\{u \in L^2(\Omega; d^n x) \,\big|\, \Delta u \in L^2(\Omega; d^n x)\big\} \tag{6.3}$$

is endowed with the natural graph norm $u \mapsto \|u\|_{L^2(\Omega;d^n x)} + \|\Delta u\|_{L^2(\Omega;d^n x)}$. *Moreover, this operator satisfies the following additional properties:*

(i) *The map* $\tau_{N,V,z}$ *in* (6.1), (6.2) *is onto* (*i.e.*, $\tau_{N,V,z}(\operatorname{dom}(H_{\max,\Omega})) = N^{1/2}(\partial\Omega)$), *for each* $z \in \mathbb{C}\backslash\sigma(H_{D,\Omega})$. *In fact,*

$$\tau_{N,V,z}\big(H^2(\Omega) \cap H^1_0(\Omega)\big) = N^{1/2}(\partial\Omega) \ \text{ for each } \ z \in \mathbb{C}\backslash\sigma(H_{D,\Omega}). \tag{6.4}$$

(ii) *One has*

$$\tau_{N,V,z} = \gamma_N (H_{D,\Omega} - zI_\Omega)^{-1}(-\Delta - z), \quad z \in \mathbb{C}\backslash\sigma(H_{D,\Omega}). \tag{6.5}$$

(iii) *For each* $z \in \mathbb{C}\backslash\sigma(H_{D,\Omega})$, *the kernel of the map* $\tau_{N,V,z}$ *in* (6.1), (6.2) *is*

$$\ker(\tau_{N,V,z}) = H^2_0(\Omega) \dot{+} \{u \in L^2(\Omega; d^n x) \,|\, (-\Delta + V - z)u = 0 \ \text{ in } \ \Omega\}. \tag{6.6}$$

In particular, if $z \in \mathbb{C}\backslash\sigma(H_{D,\Omega})$, *then*

$$\tau_{N,V,z} u = 0 \ \text{ for every } \ u \in \ker(H_{\max,\Omega} - zI_\Omega). \tag{6.7}$$

(iv) *The following Green formula holds for every* $u, v \in \operatorname{dom}(H_{\max,\Omega})$ *and every complex number* $z \in \mathbb{C}\backslash\sigma(H_{D,\Omega})$:

$$\begin{aligned} &((-\Delta + V - z)u\,,\, v)_{L^2(\Omega;d^n x)} - (u\,,\, (-\Delta + V - \overline{z})v)_{L^2(\Omega;d^n x)} \\ &\quad = -{}_{N^{1/2}(\partial\Omega)}\langle \tau_{N,V,z} u, \widehat{\gamma}_D v\rangle_{(N^{1/2}(\partial\Omega))^*} + \overline{{}_{N^{1/2}(\partial\Omega)}\langle \tau_{N,V,\overline{z}} v, \widehat{\gamma}_D u\rangle_{(N^{1/2}(\partial\Omega))^*}}. \end{aligned} \tag{6.8}$$

6.2. The perturbed Krein Laplacian in quasi-convex domains

We now discuss the Krein–von Neumann extension of the Laplacian $-\Delta\big|_{C_0^\infty(\Omega)}$ perturbed by a nonnegative, bounded potential V in $L^2(\Omega; d^n x)$. We will conveniently call this operator the *perturbed Krein Laplacian* and introduce the following basic assumption:

Hypothesis 6.2. (i) *Let $n \in \mathbb{N}$, $n \geq 2$, and assume that $\emptyset \neq \Omega \subset \mathbb{R}^n$ is a bounded Lipschitz domain satisfying Hypothesis* 5.7.
(ii) *Assume that*

$$V \in L^\infty(\Omega; d^n x) \ \text{ and } \ V \geq 0 \ \text{a.e. in } \Omega. \tag{6.9}$$

Denoting by $\overline{T}$ the closure of a linear operator T in a Hilbert space $\mathcal{H}$, we have the following result:

Lemma 6.3. *Assume Hypothesis* 6.2. *Then $H_{\min,\Omega}$ is a densely defined, closed, nonnegative* (*in particular, symmetric*) *operator in $L^2(\Omega; d^n x)$. Moreover,*

$$\overline{(-\Delta + V)\big|_{C_0^\infty(\Omega)}} = H_{\min,\Omega}. \tag{6.10}$$

Proof. The first claim in the statement is a direct consequence of Theorem 5.9. As for (6.10), let us temporarily denote by H_0 the closure of $-\Delta + V$ defined on $C_0^\infty(\Omega)$. Then

$$u \in \operatorname{dom}(H_0) \ \text{ if and only if } \begin{cases} \text{there exist } v \in L^2(\Omega; d^n x) \text{ and } u_j \in C_0^\infty(\Omega), \\ j \in \mathbb{N}, \ \text{such that } u_j \to u \ \text{ and } \ (-\Delta + V)u_j \to v \\ \text{in } \ L^2(\Omega; d^n x) \ \text{ as } \ j \to \infty. \end{cases} \tag{6.11}$$

Thus, if $u \in \operatorname{dom}(H_0)$ and v, $\{u_j\}_{j\in\mathbb{N}}$ are as in the right-hand side of (6.11), then $(-\Delta + V)u = v$ in the sense of distributions in Ω, and

$$\begin{aligned} 0 = \widehat{\gamma}_D u_j \to \widehat{\gamma}_D u \ \text{ in } \ \big(N^{1/2}(\partial\Omega)\big)^* \ \text{ as } \ j \to \infty, \\ 0 = \widehat{\gamma}_N u_j \to \widehat{\gamma}_N u \ \text{ in } \ \big(N^{1/2}(\partial\Omega)\big)^* \ \text{ as } \ j \to \infty, \end{aligned} \tag{6.12}$$

by Theorem 4.4 and Theorem 4.6. Consequently, $u \in \operatorname{dom}(H_{\max,\Omega})$ satisfies $\widehat{\gamma}_D u = 0$ and $\widehat{\gamma}_N u = 0$. Hence, $u \in H_0^2(\Omega) = \operatorname{dom}(H_{\min,\Omega})$ by Theorem 5.9 and the current assumptions on Ω. This shows that $H_0 \subseteq H_{\min,\Omega}$. The converse inclusion readily follows from the fact that any $u \in H_0^2(\Omega)$ is the limit in $H^2(\Omega)$ of a sequence of test functions in Ω. □

Lemma 6.4. *Assume Hypothesis* 6.2. *Then the Krein–von Neumann extension $H_{K,\Omega}$ of $(-\Delta + V)\big|_{C_0^\infty(\Omega)}$ in $L^2(\Omega; d^n x)$ is the L^2-realization of $-\Delta + V$ with domain*

$$\begin{aligned} \operatorname{dom}(H_{K,\Omega}) &= \operatorname{dom}(H_{\min,\Omega}) \dotplus \ker(H_{\max,\Omega}) \\ &= H_0^2(\Omega) \dotplus \big\{u \in L^2(\Omega; d^n x) \,\big|\, (-\Delta + V)u = 0 \ \text{in } \Omega\big\}. \end{aligned} \tag{6.13}$$

Proof. By virtue of (2.10), (5.20), and the fact that $(-\Delta+V)|_{C_0^\infty(\Omega)}$ and its closure, $H_{\min,\Omega}$ (cf. (6.10)) have the same self-adjoint extensions, one obtains

$$\begin{aligned}\mathrm{dom}(H_{K,\Omega}) &= \mathrm{dom}(H_{\min,\Omega}) \dotplus \ker((H_{\min,\Omega})^*) \\ &= \mathrm{dom}(H_{\min,\Omega}) \dotplus \ker(H_{\max,\Omega}) \\ &= H_0^2(\Omega) \dotplus \big\{u \in L^2(\Omega; d^n x) \,\big|\, (-\Delta+V)u = 0 \text{ in } \Omega\big\},\end{aligned} \tag{6.14}$$

as desired. □

Nonetheless, we shall adopt a different point of view which better elucidates the nature of the boundary condition associated with this perturbed Krein Laplacian. More specifically, following the same pattern as in [89], the following result can be proved.

Theorem 6.5. *Assume Hypothesis* 6.2 *and fix* $z \in \mathbb{C}\backslash\sigma(H_{D,\Omega})$. *Then* $H_{K,\Omega,z}$ *in* $L^2(\Omega; d^n x)$, *given by*

$$\begin{aligned}&H_{K,\Omega,z} u := (-\Delta + V - z)u, \\ &u \in \mathrm{dom}(H_{K,\Omega,z}) := \{v \in \mathrm{dom}(H_{\max,\Omega}) \,|\, \tau_{N,V,z} v = 0\},\end{aligned} \tag{6.15}$$

satisfies

$$(H_{K,\Omega,z})^* = H_{K,\Omega,\overline{z}}, \tag{6.16}$$

and agrees with the self-adjoint perturbed Krein Laplacian $H_{K,\Omega} = H_{K,\Omega,0}$ *when taking* $z = 0$. *In particular, if* $z \in \mathbb{R}\backslash\sigma(H_{D,\Omega})$ *then* $H_{K,\Omega,z}$ *is self-adjoint. Moreover, if* $z \leq 0$, *then* $H_{K,\Omega,z}$ *is nonnegative. Hence, the perturbed Krein Laplacian* $H_{K,\Omega}$ *is a self-adjoint operator in* $L^2(\Omega; d^n x)$ *which admits the description given in* (6.15) *when* $z = 0$, *and which satisfies*

$$H_{K,\Omega} \geq 0 \;\; \textit{and} \;\; H_{\min,\Omega} \subseteq H_{K,\Omega} \subseteq H_{\max,\Omega}. \tag{6.17}$$

Furthermore,

$$\ker(H_{K,\Omega}) = \big\{u \in L^2(\Omega; d^n x) \,\big|\, (-\Delta + V)u = 0\big\}, \tag{6.18}$$

$$\dim(\ker(H_{K,\Omega})) = \mathrm{def}(H_{\min,\Omega}) = \mathrm{def}\big(\overline{(-\Delta + V)|_{C_0^\infty(\Omega)}}\big) = \infty, \tag{6.19}$$

$$\mathrm{ran}(H_{K,\Omega}) = (-\Delta + V) H_0^2(\Omega), \tag{6.20}$$

$$H_{K,\Omega} \textit{ has a purely discrete spectrum in } (0,\infty), \quad \sigma_{\mathrm{ess}}(H_{K,\Omega}) = \{0\}, \tag{6.21}$$

and for any nonnegative self-adjoint extension $\widetilde{S}$ *of* $(-\Delta + V)|_{C_0^\infty(\Omega)}$ *one has* (*cf.* (2.5)),

$$H_{K,\Omega} \leq \widetilde{S} \leq H_{D,\Omega}. \tag{6.22}$$

The nonlocal character of the boundary condition for the Krein–von Neumann extension $H_{K,\Omega}$

$$\tau_{N,V,0} v = \widehat{\gamma}_N v + M_{D,N,\Omega,V}(0) v = 0, \quad v \in \mathrm{dom}(H_{K,\Omega}) \tag{6.23}$$

(cf. (6.15) with $z = 0$) was originally isolated by Grubb [94] (see also [95], [97]) and $M_{D,N,\Omega,V}(0)$ was identified as the operator sending Dirichlet data to Neumann data. The connection with Weyl–Titchmarsh theory and particularly, the Weyl–Titchmarsh operator $M_{D,N,\Omega,V}(z)$ (an energy-dependent Dirichlet-to-Neumann map), in the special one-dimensional half-line case $\Omega = [a,\infty)$ has been made in [180]. In terms of abstract boundary conditions in connection with the theory of boundary value spaces, such a Weyl–Titchmarsh connection has also been made in [67] and [68]. However, we note that this abstract boundary value space approach, while applicable to ordinary differential operators, is not applicable to partial differential operators even in the case of smooth boundaries $\partial\Omega$ (see, e.g., the discussion in [35]). In particular, it does not apply to the nonsmooth domains Ω studied in this survey. In fact, only very recently, appropriate modifications of the theory of boundary value spaces have successfully been applied to partial differential operators in smooth domains in [35], [50], [51], [52], [158], [159], [164], [165], and [166]. With the exception of the following short discussions: Subsection 4.1 in [35] (which treat the special case where Ω equals the unit ball in $\mathbb{R}^2$), Remark 3.8 in [50], Section 2 in [164], Subsection 2.4 in [165], and Remark 5.12 in [166], these investigations did not enter a detailed discussion of the Krein-von Neumann extension. In particular, none of these references applies to the case of nonsmooth domains Ω.

7. Connections with the problem of the buckling of a clamped plate

In this section we proceed to study a fourth-order problem, which is a perturbation of the classical problem for the buckling of a clamped plate, and which turns out to be essentially spectrally equivalent to the perturbed Krein Laplacian $H_{K,\Omega} := H_{K,\Omega,0}$.

For now, let us assume Hypotheses 4.1 and 4.7. Given $\lambda \in \mathbb{C}$, consider the eigenvalue problem for the generalized buckling of a clamped plate in the domain $\Omega \subset \mathbb{R}^n$

$$\begin{cases} u \in \operatorname{dom}(-\Delta_{\max,\Omega}), \\ (-\Delta + V)^2 u = \lambda\,(-\Delta + V)u \ \text{ in } \ \Omega, \\ \widehat{\gamma}_D u = 0 \ \text{ in } \ \big(N^{1/2}(\partial\Omega)\big)^*, \\ \widehat{\gamma}_N u = 0 \ \text{ in } \ \big(N^{3/2}(\partial\Omega)\big)^*, \end{cases} \tag{7.1}$$

where $(-\Delta+V)^2u := (-\Delta+V)(-\Delta u+Vu)$ in the sense of distributions in Ω. Due to the trace theory developed in Sections 4 and 5, this formulation is meaningful. In addition, if Hypothesis 5.7 is assumed in place of Hypothesis 4.1 then, by (4.66), this problem can be equivalently rephrased as

$$\begin{cases} u \in H_0^2(\Omega), \\ (-\Delta + V)^2 u = \lambda\,(-\Delta + V)u \ \text{ in } \ \Omega. \end{cases} \tag{7.2}$$

Lemma 7.1. *Assume Hypothesis* 6.2 *and suppose that* $u \neq 0$ *solves* (7.1) *for some* $\lambda \in \mathbb{C}$. *Then necessarily* $\lambda \in (0,\infty)$.

Proof. Let u, λ be as in the statement of the lemma. Then, as already pointed out above, $u \in H_0^2(\Omega)$. Based on this, the fact that $\Delta u \in \mathrm{dom}(-\Delta_{\max,\Omega})$, and the integration by parts formulas (4.21) and (4.35), we may then write (we recall that our L^2 pairing is conjugate linear in the *first* argument):

$$\begin{aligned}
&\lambda\big[\|\nabla u\|^2_{(L^2(\Omega;d^nx))^n} + \|V^{1/2}u\|^2_{(L^2(\Omega;d^nx))^n}\big] = \lambda\,(u,(-\Delta+V)u)_{L^2(\Omega;d^nx)}\\
&\quad = (u\,,\,\lambda\,(-\Delta+V)u)_{L^2(\Omega;d^nx)} = \big(u,(-\Delta+V)^2u\big)_{L^2(\Omega;d^nx)}\\
&\quad = (u,(-\Delta+V)(-\Delta u+Vu))_{L^2(\Omega;d^nx)} = ((-\Delta+V)u,(-\Delta+V)u)_{L^2(\Omega;d^nx)}\\
&\quad = \|(-\Delta+V)u\|^2_{L^2(\Omega;d^nx)}. \qquad (7.3)
\end{aligned}$$

Since, according to Theorem 5.11, $L^2(\Omega;d^nx) \ni u \neq 0$ and $\widehat{\gamma}_D u = 0$ prevent u from being a constant function, (7.3) entails

$$\lambda = \frac{\|(-\Delta+V)u\|^2_{L^2(\Omega;d^nx)}}{\|\nabla u\|^2_{(L^2(\Omega;d^nx))^n} + \|V^{1/2}u\|^2_{(L^2(\Omega;d^nx))^n}} > 0, \qquad (7.4)$$

as desired. □

Next, we recall the operator $P_{D,\Omega,V,z}$ introduced just above (5.26) and agree to simplify notation by abbreviating $P_{D,\Omega,V} := P_{D,\Omega,V,0}$. That is,

$$P_{D,\Omega,V} = \big[\gamma_N(H_{D,\Omega})^{-1}\big]^* \in \mathcal{B}\big((N^{1/2}(\partial\Omega))^*, L^2(\Omega;d^nx)\big) \qquad (7.5)$$

is such that if $u := P_{D,\Omega,V}\,g$ for some $g \in \big(N^{1/2}(\partial\Omega)\big)^*$, then

$$\begin{cases} (-\Delta+V)u = 0 \text{ in } \Omega,\\ u \in L^2(\Omega;d^nx),\\ \widehat{\gamma}_D u = g \text{ on } \partial\Omega. \end{cases} \qquad (7.6)$$

Hence,

$$\begin{aligned}
&(-\Delta+V)P_{D,\Omega,V} = 0,\\
&\widehat{\gamma}_N P_{D,\Omega,V} = -M_{D,N,\Omega,V}(0) \text{ and } \widehat{\gamma}_D P_{D,\Omega,V} = I_{(N^{1/2}(\partial\Omega))^*},
\end{aligned} \qquad (7.7)$$

with $I_{(N^{1/2}(\partial\Omega))^*}$ the identity operator, on $\big(N^{1/2}(\partial\Omega)\big)^*$.

Theorem 7.2. *Assume Hypothesis* 6.2. *If* $0 \neq v \in L^2(\Omega;d^nx)$ *is an eigenfunction of the perturbed Krein Laplacian* $H_{K,\Omega}$ *corresponding to the eigenvalue* $0 \neq \lambda \in \mathbb{C}$ (*hence* $\lambda > 0$)*, then*

$$u := v - P_{D,\Omega,V}(\widehat{\gamma}_D v) \qquad (7.8)$$

is a nontrivial solution of (7.1). *Conversely, if* $0 \neq u \in L^2(\Omega;d^nx)$ *solves* (7.1) *for some* $\lambda \in \mathbb{C}$ *then* λ *is a* (*strictly*) *positive eigenvalue of the perturbed Krein Laplacian* $H_{K,\Omega}$*, and*

$$v := \lambda^{-1}(-\Delta+V)u \qquad (7.9)$$

is a nonzero eigenfunction of the perturbed Krein Laplacian, corresponding to this eigenvalue.

Proof. In one direction, assume that $0 \neq v \in L^2(\Omega; d^n x)$ is an eigenfunction of the perturbed Krein Laplacian $H_{K,\Omega}$ corresponding to the eigenvalue $0 \neq \lambda \in \mathbb{C}$ (since $H_{K,\Omega} \geq 0$ – cf. Theorem 6.5 – it follows that $\lambda > 0$). Thus, v satisfies

$$v \in \operatorname{dom}(H_{\max,\Omega}), \quad (-\Delta + V)v = \lambda\, v, \ \tau_{N,V,0} v = 0. \tag{7.10}$$

In particular, $\widehat{\gamma}_D v \in \big(N^{1/2}(\partial\Omega)\big)^*$ by Theorem 4.4. Hence, by (7.5), u in (7.8) is a well-defined function which belongs to $L^2(\Omega; d^n x)$. In fact, since also $(-\Delta+V)u = (-\Delta+V)v \in L^2(\Omega; d^n x)$, it follows that $u \in \operatorname{dom}(H_{\max,\Omega})$. Going further, we note that

$$\begin{aligned}(-\Delta + V)^2 u &= (-\Delta + V)(-\Delta + V)u = (-\Delta + V)(-\Delta + V)v \\ &= \lambda\,(-\Delta + V)v = \lambda\,(-\Delta + V)u.\end{aligned} \tag{7.11}$$

Hence, $(-\Delta + V)^2 u = \lambda\,(-\Delta + V)u$ in Ω. In addition, by (7.7),

$$\widehat{\gamma}_D u = \widehat{\gamma}_D v - \widehat{\gamma}_D (P_{D,\Omega,V}(\widehat{\gamma}_D v) = \widehat{\gamma}_D v - \widehat{\gamma}_D v = 0, \tag{7.12}$$

whereas

$$\widehat{\gamma}_N u = \widehat{\gamma}_N v - \widehat{\gamma}_N (P_{D,\Omega,V}(\widehat{\gamma}_D v) = \widehat{\gamma}_N v + M_{D,N,\Omega,V}(0)(\widehat{\gamma}_D v) = \tau_{N,V,0} v = 0, \tag{7.13}$$

by the last condition in (7.10). Next, to see that u cannot vanish identically, we note that $u = 0$ would imply $v = P_{D,\Omega,V}(\widehat{\gamma}_D v)$ which further entails $\lambda\, v = (-\Delta + V)v = (-\Delta + V)P_{D,\Omega,V}(\widehat{\gamma}_D v) = 0$, that is, $v = 0$ (since $\lambda \neq 0$). This contradicts the original assumption on v and shows that u is a nontrivial solution of (7.1). This completes the proof of the first half of the theorem.

Turning to the second half, suppose that $\lambda \in \mathbb{C}$ and $0 \neq u \in L^2(\Omega; d^n x)$ is a solution of (7.1). Lemma 7.1 then yields $\lambda > 0$, so that $v := \lambda^{-1}(-\Delta + V)u$ is a well-defined function satisfying

$$v \in \operatorname{dom}(H_{\max,\Omega}) \ \text{ and } \ (-\Delta+V)v = \lambda^{-1}\,(-\Delta+V)^2 u = (-\Delta+V)u = \lambda\, v. \tag{7.14}$$

If we now set $w := v - u \in L^2(\Omega; d^n x)$ it follows that

$$(-\Delta + V)w = (-\Delta + V)v - (-\Delta + V)u = \lambda\, v - \lambda\, v = 0, \tag{7.15}$$

and

$$\widehat{\gamma}_N w = \widehat{\gamma}_N v, \quad \widehat{\gamma}_D w = \widehat{\gamma}_D v. \tag{7.16}$$

In particular, by the uniqueness in the Dirichlet problem (7.6),

$$w = P_{D,\Omega,V}(\widehat{\gamma}_D v). \tag{7.17}$$

Consequently,

$$\widehat{\gamma}_N v = \widehat{\gamma}_N w = \widehat{\gamma}_N (P_{D,\Omega,V}(\widehat{\gamma}_D v) = -M_{D,N,\Omega,V}(0)(\widehat{\gamma}_D v), \tag{7.18}$$

which shows that

$$\tau_{N,V,0} v = \widehat{\gamma}_N v + M_{D,N,\Omega,V}(0)(\widehat{\gamma}_D v) = 0. \tag{7.19}$$

Hence $v \in \operatorname{dom}(H_{K,\Omega})$. We note that $v = 0$ would entail that the function $u \in H^2_0(\Omega)$ is a null solution of $-\Delta + V$, hence identically zero which, by assumption, is not the case. Therefore, v does not vanish identically. Altogether, the above reasoning shows that v is a nonzero eigenfunction of the perturbed Krein Laplacian, corresponding to the positive eigenvalue $\lambda > 0$, completing the proof. $\square$

Proposition 7.3.

(i) *Assume Hypothesis* 6.2 *and let* $0 \neq v$ *be any eigenfunction of* $H_{K,\Omega}$ *corresponding to the eigenvalue* $0 \neq \lambda \in \sigma(H_{K,\Omega})$. *In addition suppose that the operator of multiplication by* V *satisfies*

$$M_V \in \mathcal{B}\big(H^2(\Omega), H^s(\Omega)\big) \text{ for some } 1/2 < s \leq 2. \tag{7.20}$$

Then u *defined in* (7.8) *satisfies*

$$u \in H^{5/2}(\Omega), \text{ implying } v \in H^{1/2}(\Omega). \tag{7.21}$$

(ii) *Assume the smooth case, that is,* $\partial\Omega$ *is* C^∞ *and* $V \in C^\infty(\overline{\Omega})$, *and let* $0 \neq v$ *be any eigenfunction of* $H_{K,\Omega}$ *corresponding to the eigenvalue* $0 \neq \lambda \in \sigma(H_{K,\Omega})$. *Then* u *defined in* (7.8) *satisfies*

$$u \in C^\infty(\overline{\Omega}), \text{ implying } v \in C^\infty(\overline{\Omega}). \tag{7.22}$$

Proof. (i) We note that $u \in L^2(\Omega; d^n x)$ satisfies $\widehat{\gamma}_D(u) = 0$, $\widehat{\gamma}_N(u) = 0$, and $(-\Delta + V)u = (-\Delta + V)v = \lambda v \in L^2(\Omega; d^n x)$. Hence, by Theorems 5.9 and 5.11, we obtain that $u \in H_0^2(\Omega)$. Next, observe that $(-\Delta + V)^2 u = \lambda^2 v \in L^2(\Omega; d^n x)$ which therefore entails $\Delta^2 u \in H^{s-2}(\Omega)$ by (7.20). With this at hand, the regularity results in [157] (cf. also [5] for related results) yield that $u \in H^{5/2}(\Omega)$.

(ii) Given the eigenfunction $0 \neq v$ of $H_{K,\Omega}$, (7.8) yields that u satisfies the generalized buckling problem (7.1), so that by elliptic regularity $u \in C^\infty(\overline{\Omega})$. By (7.9) and (7.10) one thus obtains

$$\lambda v = (-\Delta + V)v = (-\Delta + V)u, \text{ with } u \in C^\infty(\overline{\Omega}), \tag{7.23}$$

proving (7.22). $\square$

In passing, we note that the multiplier condition (7.20) is satisfied, for instance, if V is Lipschitz.

We next wish to prove that the perturbed Krein Laplacian has only point spectrum (which, as the previous theorem shows, is directly related to the eigenvalues of the generalized buckling of the clamped plate problem). This requires some preparations, and we proceed by first establishing the following.

Lemma 7.4. *Assume Hypothesis* 6.2. *Then there exists a discrete subset* Λ_Ω *of* $(0, \infty)$ *without any finite accumulation points which has the following significance: For every* $z \in \mathbb{C}\backslash\Lambda_\Omega$ *and every* $f \in H^{-2}(\Omega)$, *the problem*

$$\begin{cases} u \in H_0^2(\Omega), \\ (-\Delta + V)(-\Delta + V - z)u = f \text{ in } \Omega, \end{cases} \tag{7.24}$$

has a unique solution. In addition, there exists $C = C(\Omega, z) > 0$ *such that the solution satisfies*

$$\|u\|_{H^2(\Omega)} \leq C\|f\|_{H^{-2}(\Omega)}. \tag{7.25}$$

Finally, if $z \in \Lambda_\Omega$, then there exists $u \neq 0$ satisfying (7.2). *In fact, the space of solutions for the problem* (7.2) *is, in this case, finite dimensional and nontrivial.*

Proof. In a first stage, fix $z \in \mathbb{C}$ with $\operatorname{Re}(z) \leq -M$, where $M = M(\Omega, V) > 0$ is a large constant to be specified later, and consider the bounded sesquilinear form

$$\begin{aligned} a_{V,z}(\,\cdot\,,\,\cdot\,) :& H_0^2(\Omega) \times H_0^2(\Omega) \to \mathbb{C}, \\ a_{V,z}(u,v) :=& ((-\Delta+V)u, (-\Delta+V)v)_{L^2(\Omega;d^nx)} + \big(V^{1/2}u, V^{1/2}v\big)_{L^2(\Omega;d^nx)} \\ &- z\,(\nabla u, \nabla v)_{(L^2(\Omega;d^nx))^n}, \quad u,v \in H_0^2(\Omega). \end{aligned} \tag{7.26}$$

Then, since $f \in H^{-2}(\Omega) = \big(H_0^2(\Omega)\big)^*$, the well-posedness of (7.24) will follow with the help of the Lax-Milgram lemma as soon as we show that (7.26) is coercive. To this end, observe that via repeated integrations by parts

$$\begin{aligned} a_{V,z}(u,u) = &\sum_{j,k=1}^n \int_\Omega d^nx\, \bigg|\frac{\partial^2 u}{\partial x_j \partial x_k}\bigg|^2 - z\sum_{j=1}^n \int_\Omega d^nx\, \bigg|\frac{\partial u}{\partial x_j}\bigg|^2 \\ &+ \int_\Omega d^nx\, \big|V^{1/2}u\big| + 2\operatorname{Re}\bigg(\int_\Omega d^nx\, \Delta u\, V\overline{u}\bigg), \quad u \in C_0^\infty(\Omega). \end{aligned} \tag{7.27}$$

We note that the last term is of the order

$$O\big(\|V\|_{L^\infty(\Omega;d^nx)}\|\Delta u\|_{L^2(\Omega;d^nx)}\|u\|_{L^2(\Omega;d^nx)}\big) \tag{7.28}$$

and hence, can be dominated by

$$C\|V\|_{L^\infty(\Omega;d^nx)}\big[\varepsilon\|u\|^2_{H^2(\Omega)} + (4\varepsilon)^{-1}\|u\|^2_{L^2(\Omega;d^nx)}\big], \tag{7.29}$$

for every $\varepsilon > 0$. Thus, based on this and Poincaré's inequality, we eventually obtain, by taking $\varepsilon > 0$ sufficiently small, and M (introduced in the beginning of the proof) sufficiently large, that

$$\operatorname{Re}(a_{V,z}(u,u)) \geq C\|u\|^2_{H^2(\Omega)}, \quad u \in C_0^\infty(\Omega). \tag{7.30}$$

Hence,

$$\operatorname{Re}(a_{V,z}(u,u)) \geq C\|u\|^2_{H^2(\Omega)}, \quad u \in H_0^2(\Omega), \tag{7.31}$$

by the density of $C_0^\infty(\Omega)$ in $H_0^2(\Omega)$. Thus, the form (7.27) is coercive and hence, the problem (7.24) is well posed whenever $z \in \mathbb{C}$ has $\operatorname{Re}(z) \leq -M$.

We now wish to extend this type of conclusion to a larger set of z's. With this in mind, set

$$A_{V,z} := (-\Delta+V)(-\Delta+V-zI_\Omega) \in \mathcal{B}\big(H_0^2(\Omega), H^{-2}(\Omega)\big), \quad z \in \mathbb{C}. \tag{7.32}$$

The well-posedness of (7.24) is equivalent to the fact that the above operator is invertible. In this vein, we note that if we fix $z_0 \in \mathbb{C}$ with $\operatorname{Re}(z_0) \leq -M$, then, from what we have shown so far,

$$A^{-1}_{V,z_0} \in \mathcal{B}\big(H^{-2}(\Omega), H_0^2(\Omega)\big) \tag{7.33}$$

is a well-defined operator. For an arbitrary $z \in \mathbb{C}$ we then write

$$A_{V,z} = A_{V,z_0}[I_{H_0^2(\Omega)} + B_{V,z}], \tag{7.34}$$

where $I_{H_0^2(\Omega)}$ is the identity operator on $H_0^2(\Omega)$ and we have set

$$B_{V,z} := A_{V,z_0}^{-1}(A_{V,z} - A_{V,z_0}) = (z_0 - z)A_{V,z_0}^{-1}(-\Delta + V) \in \mathcal{B}_\infty\big(H_0^2(\Omega)\big). \quad (7.35)$$

Since $\mathbb{C} \ni z \mapsto B_{V,z} \in \mathcal{B}\big(H_0^2(\Omega)\big)$ is an analytic, compact operator-valued mapping, which vanishes for $z = z_0$, the Analytic Fredholm Theorem yields the existence of an exceptional, discrete set $\Lambda_\Omega \subset \mathbb{C}$, without any finite accumulation points such that

$$(I_{H_0^2(\Omega)} + B_{V,z})^{-1} \in \mathcal{B}\big(H_0^2(\Omega)\big), \quad z \in \mathbb{C}\backslash\Lambda_\Omega. \quad (7.36)$$

As a consequence of this, (7.33), and (7.34), we therefore have

$$A_{V,z}^{-1} \in \mathcal{B}\big(H^{-2}(\Omega), H_0^2(\Omega)\big), \quad z \in \mathbb{C}\backslash\Lambda_\Omega. \quad (7.37)$$

We now proceed to show that, in fact, $\Lambda_\Omega \subset (0,\infty)$. To justify this inclusion, we observe that

$$\begin{array}{l} A_{V,z} \text{ in (7.32) is a Fredholm operator, with} \\ \text{Fredholm index zero, for every } z \in \mathbb{C}, \end{array} \quad (7.38)$$

due to (7.33), (7.34), and (7.35). Thus, if for some $z \in \mathbb{C}$ the operator $A_{V,z}$ fails to be invertible, then there exists $0 \neq u \in L^2(\Omega; d^n x)$ such that $A_{V,z}u = 0$. In view of (7.32) and Lemma 7.1, the latter condition forces $z \in (0,\infty)$. Thus, Λ_Ω consists of positive numbers. At this stage, it remains to justify the very last claim in the statement of the lemma. This, however, readily follows from (7.38), completing the proof. □

Theorem 7.5. *Assume Hypothesis* 6.2 *and recall the exceptional set* $\Lambda_\Omega \subset (0,\infty)$ *from Lemma* 7.4, *which is discrete with only accumulation point at infinity. Then*

$$\sigma(H_{K,\Omega}) = \Lambda_\Omega \cup \{0\}. \quad (7.39)$$

Furthermore, for every $0 \neq z \in \mathbb{C}\backslash\Lambda_\Omega$, *the action of the resolvent* $(H_{K,\Omega} - zI_\Omega)^{-1}$ *on an arbitrary element* $f \in L^2(\Omega; d^n x)$ *can be described as follows: Let* v *solve*

$$\begin{cases} v \in H_0^2(\Omega), \\ (-\Delta + V)(-\Delta + V - z)v = (-\Delta + V)f \in H^{-2}(\Omega), \end{cases} \quad (7.40)$$

and consider

$$w := z^{-1}[(-\Delta + V - z)v - f] \in L^2(\Omega; d^n x). \quad (7.41)$$

Then

$$(H_{K,\Omega} - zI_\Omega)^{-1} f = v + w. \quad (7.42)$$

Finally, every $z \in \Lambda_\Omega \cup \{0\}$ *is actually an eigenvalue* (*of finite multiplicity, if nonzero*) *for the perturbed Krein Laplacian, and the essential spectrum of this operator is given by*

$$\sigma_{ess}(H_{K,\Omega}) = \{0\}. \quad (7.43)$$

Proof. Let $0 \neq z \in \mathbb{C}\backslash\Lambda_\Omega$, fix $f \in L^2(\Omega; d^n x)$, and assume that v, w are as in the statement of the theorem. That v (hence also w) is well defined follows from Lemma 7.4. Set

$$\begin{aligned} u := v + w \in & H_0^2(\Omega) \dot{+} \big\{\eta \in L^2(\Omega; d^n x) \,\big|\, (-\Delta + V)\eta = 0 \text{ in } \Omega\big\} \\ & = \ker\big(\tau_{N,V,0}\big) \hookrightarrow \operatorname{dom}(H_{\max,\Omega}), \end{aligned} \tag{7.44}$$

by (6.6). Thus, $u \in \operatorname{dom}(H_{\max,\Omega})$ and $\tau_{N,V,0} u = 0$ which force $u \in \operatorname{dom}(H_{K,\Omega})$. Furthermore,

$$\|u\|_{L^2(\Omega; d^n x)} + \|\Delta u\|_{L^2(\Omega; d^n x)} \leq C\|f\|_{L^2(\Omega; d^n x)}, \tag{7.45}$$

for some $C = C(\Omega, V, z) > 0$, and

$$\begin{aligned} (-\Delta + V - z)u &= (-\Delta + V - z)v + (-\Delta + V - z)w \\ &= (-\Delta + V - z)v + z^{-1}(-\Delta + V - z)[(-\Delta + V - z)v - f] \\ &= (-\Delta + V - z)v + z^{-1}(-\Delta + V)[(-\Delta + V - z)v - f] - [(-\Delta + V - z)v - f] \\ &= f + z^{-1}[(-\Delta + V)(-\Delta + V - z)v - (-\Delta + V)f] = f, \end{aligned} \tag{7.46}$$

by (7.40), (7.41). As a consequence of this analysis, we may conclude that the operator

$$H_{K,\Omega} - zI_\Omega : \operatorname{dom}(H_{K,\Omega}) \subset L^2(\Omega; d^n x) \to L^2(\Omega; d^n x) \tag{7.47}$$

is onto (with norm control), for every $z \in \mathbb{C}\backslash(\Lambda_\Omega \cup \{0\})$. When $z \in \mathbb{C}\backslash(\Lambda_\Omega \cup \{0\})$ the last part in Lemma 7.4 together with Theorem 7.2 also yield that the operator (7.47) is injective. Together, these considerations prove that

$$\sigma(H_{K,\Omega}) \subseteq \Lambda_\Omega \cup \{0\}. \tag{7.48}$$

Since the converse inclusion also follows from the last part in Lemma 7.4 together with Theorem 7.2, equality (7.39) follows. Formula (7.42), along with the final conclusion in the statement of the theorem, is also implicit in the above analysis plus the fact that $\ker(H_{K,\Omega})$ is infinite dimensional (cf. (2.46) and [145]). □

8. Eigenvalue estimates for the perturbed Krein Laplacian

The aim of this section is to study in greater detail the nature of the spectrum of the operator $H_{K,\Omega}$. We split the discussion into two separate cases, dealing with the situation when the potential V is as in Hypothesis 4.7 (Subsection 8.1), and when $V \equiv 0$ (Subsection 8.2).

8.1. The perturbed case

Given a domain Ω as in Hypothesis 5.7 and a potential V as in Hypothesis 4.7, we recall the exceptional set $\Lambda_\Omega \subset (0, \infty)$ associated with Ω as in Section 7, consisting of numbers

$$0 < \lambda_{K,\Omega,1} \leq \lambda_{K,\Omega,2} \leq \cdots \leq \lambda_{K,\Omega,j} \leq \lambda_{K,\Omega,j+1} \leq \cdots \tag{8.1}$$

converging to infinity. Above, we have displayed the λ's according to their (geometric) multiplicity which equals the dimension of the kernel of the (Fredholm) operator (7.32).

Lemma 8.1. *Assume Hypothesis* 6.2. *Then there exists a family of functions* $\{u_j\}_{j\in\mathbb{N}}$ *with the following properties:*

$$u_j \in H_0^2(\Omega) \text{ and } (-\Delta+V)^2 u_j = \lambda_{K,\Omega,j}(-\Delta+V)u_j, \quad j\in\mathbb{N}, \tag{8.2}$$

$$((-\Delta+V)u_j, (-\Delta+V)u_k)_{L^2(\Omega;d^nx)} = \delta_{j,k}, \quad j,k\in\mathbb{N}, \tag{8.3}$$

$$u = \sum_{j=1}^{\infty} ((-\Delta+V)u, (-\Delta+V)u_j)_{L^2(\Omega;d^nx)}\, u_j, \quad u \in H_0^2(\Omega), \tag{8.4}$$

with convergence in $H^2(\Omega)$.

Proof. Consider the vector space and inner product

$$\mathcal{H}_V := H_0^2(\Omega), \quad [u,v]_{\mathcal{H}_V} := \int_\Omega d^nx\, \overline{(-\Delta+V)u}\,(-\Delta+V)v, \quad u,v\in\mathcal{H}_V. \tag{8.5}$$

We claim that $\big(\mathcal{H}_V, [\,\cdot\,,\,\cdot\,]_{\mathcal{H}_V}\big)$ is a Hilbert space. This readily follows as soon as we show that

$$\|u\|_{H^2(\Omega)} \leq C\|(-\Delta+V)u\|_{L^2(\Omega;d^nx)}, \quad u\in H_0^2(\Omega), \tag{8.6}$$

for some finite constant $C=C(\Omega,V)>0$. To justify this, observe that for every $u\in C_0^\infty(\Omega)$ we have

$$\begin{aligned}\int_\Omega d^nx\,|u|^2 &\leq C\sum_{j=1}^n \int_\Omega d^nx\,\left|\frac{\partial u}{\partial x_j}\right|^2 \\ &\leq C\sum_{j,k=1}^n \int_\Omega d^nx\,\left|\frac{\partial^2 u}{\partial x_j\partial x_k}\right|^2 = \int_\Omega d^nx\,|\Delta u|^2,\end{aligned} \tag{8.7}$$

where we have used Poincaré's inequality in the first two steps. Based on this, the fact that V is bounded, and the density of $C_0^\infty(\Omega)$ in $H_0^2(\Omega)$ we therefore have

$$\|u\|_{H^2(\Omega)} \leq C\big(\|(-\Delta+V)u\|_{L^2(\Omega;d^nx)} + \|u\|_{L^2(\Omega;d^nx)}\big), \quad u\in H_0^2(\Omega), \tag{8.8}$$

for some finite constant $C=C(\Omega,V)>0$. Hence, the operator

$$-\Delta+V \in \mathcal{B}\big(H_0^2(\Omega), L^2(\Omega;d^nx)\big) \tag{8.9}$$

is bounded from below modulo compact operators, since the embedding $H_0^2(\Omega)\hookrightarrow L^2(\Omega;d^nx)$ is compact. Hence, it follows that (8.9) has closed range. Since this operator is also one-to-one (as $0\notin\sigma(H_{D,\Omega})$), estimate (8.6) follows from the Open Mapping Theorem. This shows that

$$\mathcal{H}_V = H_0^2(\Omega) \text{ as Banach spaces, with equivalence of norms.} \tag{8.10}$$

Next, we recall from the proof of Lemma 7.4 that the operator (7.32) is invertible for $\lambda\in\mathbb{C}\backslash\Lambda_\Omega$ (cf. (7.37)), and that $\Lambda_\Omega\subset(0,\infty)$. Taking $\lambda=0$ this shows that

$$(-\Delta+V)^{-2} := ((-\Delta+V)^2)^{-1} \in \mathcal{B}\big(H^{-2}(\Omega), H_0^2(\Omega)\big) \tag{8.11}$$

is well defined. Furthermore, this operator is self-adjoint (viewed as a linear, bounded operator mapping a Banach space into its dual, cf. (2.1)). Consider now

$$B := -(-\Delta + V)^{-2}(-\Delta + V). \tag{8.12}$$

Since B admits the factorization

$$B : H_0^2(\Omega) \xrightarrow{-\Delta+V} L^2(\Omega; d^n x) \overset{\iota}{\hookrightarrow} H^{-2}(\Omega) \xrightarrow{-(-\Delta+V)^{-2}} H_0^2(\Omega), \tag{8.13}$$

where the middle arrow is a compact inclusion, it follows that

$$B \in \mathcal{B}(\mathcal{H}_V) \text{ is compact and injective.} \tag{8.14}$$

In addition, for every $u, v \in C_0^\infty(\Omega)$ we have via repeated integrations by parts

$$\begin{aligned}
[Bu, v]_{\mathcal{H}_V} &= -\big((-\Delta + V)(-\Delta + V)^{-2}(-\Delta + V)u, (-\Delta + V)v\big)_{L^2(\Omega;d^n x)} \\
&= -\big((-\Delta + V)^{-2}(-\Delta + V)u, (-\Delta + V)^2 v\big)_{L^2(\Omega;d^n x)} \\
&= -\big((-\Delta + V)u, (-\Delta + V)^{-2}(-\Delta + V)^2 v\big)_{L^2(\Omega;d^n x)} \\
&= -((-\Delta + V)u, v)_{L^2(\Omega;d^n x)} \\
&= -(\nabla u, \nabla v)_{(L^2(\Omega;d^n x))^n} - \big(V^{1/2}u, V^{1/2}v\big)_{L^2(\Omega;d^n x)}.
\end{aligned} \tag{8.15}$$

Consequently, by symmetry, $[Bu, v]_{\mathcal{H}_V} = \overline{[Bv, u]_{\mathcal{H}_V}}$, $u, v \in C_0^\infty(\Omega)$ and hence,

$$[Bu, v]_{\mathcal{H}_V} = \overline{[Bv, u]_{\mathcal{H}_V}} \quad u, v \in \mathcal{H}_V, \tag{8.16}$$

since $C_0^\infty(\Omega) \hookrightarrow \mathcal{H}_V$ densely. Thus,

$$B \in \mathcal{B}_\infty(\mathcal{H}_V) \text{ is self-adjoint and injective.} \tag{8.17}$$

To continue, we recall the operator $A_{V,\lambda}$ from (7.32) and observe that

$$(-\Delta + V)^{-2} A_{V,z} = I_{\mathcal{H}_V} - zB, \quad z \in \mathbb{C}, \tag{8.18}$$

as operators in $\mathcal{B}\big(H_0^2(\Omega)\big)$. Thus, the spectrum of B consists (including multiplicities) precisely of the reciprocals of those numbers $z \in \mathbb{C}$ for which the operator $A_{V,z} \in \mathcal{B}\big(H_0^2(\Omega), H^{-2}(\Omega)\big)$ fails to be invertible. In other words, the spectrum of $B \in \mathcal{B}(\mathcal{H}_V)$ is given by

$$\sigma(B) = \{(\lambda_{K,\Omega,j})^{-1}\}_{j\in\mathbb{N}}. \tag{8.19}$$

Now, from the spectral theory of compact, self-adjoint (injective) operators on Hilbert spaces (cf., e.g., [142, Theorem 2.36]), it follows that there exists a family of functions $\{u_j\}_{j\in\mathbb{N}}$ for which

$$u_j \in \mathcal{H}_V \text{ and } Bu_j = (\lambda_{K,\Omega,j})^{-1} u_j, \quad j \in \mathbb{N}, \tag{8.20}$$

$$[u_j, u_k]_{\mathcal{H}_V} = \delta_{j,k}, \quad j, k \in \mathbb{N}, \tag{8.21}$$

$$u = \sum_{j=1}^{\infty} [u, u_j]_{\mathcal{H}_V}\, u_j, \quad u \in \mathcal{H}_V, \tag{8.22}$$

with convergence in $\mathcal{H}_V$. Unraveling notation, (8.2)–(8.4) then readily follow from (8.20)–(8.22). □

Remark 8.2. We note that Lemma 8.1 gives the orthogonality of the eigenfunctions u_j in terms of the inner product for $\mathcal{H}_V$ (cf. (8.3) and (8.5), or see (8.21) immediately above). Here we remark that the given inner product for $\mathcal{H}_V$ does not correspond to the inner product that has traditionally been used in treating the buckling problem for a clamped plate, even after specializing to the case $V \equiv 0$. The traditional inner product in that case is the *Dirichlet inner product*, defined by

$$D(u,v) = \int_\Omega d^n x \, (\nabla u, \nabla v)_{\mathbb{C}^n}, \quad u,v \in H_0^1(\Omega), \tag{8.23}$$

where $(\cdot,\cdot)_{\mathbb{C}^n}$ denotes the usual inner product for elements of $\mathbb{C}^n$, conjugate linear in its first entry, linear in its second. When the potential $V \geqslant 0$ is included, the appropriate generalization of $D(u,v)$ is the inner product

$$D_V(u,v) = D(u,v) + \int_\Omega d^n x \, V \overline{u} \, v, \quad u,v \in H_0^1(\Omega) \tag{8.24}$$

(we recall that throughout this survey V is assumed nonnegative, and hence that this inner product gives rise to a well-defined norm). Here we observe that orthogonality of the eigenfunctions of the buckling problem in the sense of $\mathcal{H}_V$ is entirely equivalent to their orthogonality in the sense of $D_V(\cdot,\cdot)$: Indeed, starting from the orthogonality in (8.21), integrating by parts, and using the eigenvalue equation (8.2), one has, for $j \neq k$,

$$\begin{aligned} 0 = [u_j, u_k]_{\mathcal{H}_V} &= \int_\Omega d^n x \, \overline{(-\Delta + V) u_j} \, (-\Delta + V) u_k = \int_\Omega d^n x \, \overline{u_j} \, (-\Delta + V)^2 u_k \\ &= \lambda_k \int_\Omega d^n x \, \overline{u_j} \, (-\Delta + V) u_k = \lambda_k \bigg[D(u_j, u_k) + \int_\Omega d^n x \, V \overline{u_j} \, u_k \bigg] \\ &= \lambda_k \, D_V(u_j, u_k), \quad u,v \in H_0^2(\Omega), \end{aligned} \tag{8.25}$$

where λ_k is shorthand for $\lambda_{K,\Omega,k}$ of (8.1), the eigenvalue corresponding to the eigenfunction u_k (cf. (8.2), which exhibits the eigenvalue equation for the eigenpair (u_j, λ_j)). Since all the λ_j's considered here are positive (see (8.1)), this shows that the family of eigenfunctions $\{u_j\}_{j \in \mathbb{N}}$, orthogonal with respect to $[\cdot,\cdot]_{\mathcal{H}_V}$, is also orthogonal with respect to the "generalized Dirichlet inner product", $D_V(\cdot,\cdot)$. Clearly, this argument can also be reversed (since all eigenvalues are positive), and one sees that a family of eigenfunctions of the generalized buckling problem orthogonal in the sense of the Dirichlet inner product $D_V(\cdot,\cdot)$ is also orthogonal with respect to the inner product for $\mathcal{H}_V$, that is, with respect to $[\cdot,\cdot]_{\mathcal{H}_V}$. On the other hand, it should be mentioned that the normalization of each of the u_k's changes if one passes from one of these inner products to the other, due to the factor of λ_k encountered above (specifically, one has $[u_k, u_k]_{\mathcal{H}_V} = \lambda_k \, D_V(u_k, u_k)$ for each k).

Next, we recall the following result (which provides a slight variation of the case $V \equiv 0$ treated in [89]).

Lemma 8.3. *Assume Hypothesis* 6.2. *Then the subspace* $(-\Delta+V)\,H_0^2(\Omega)$ *is closed in* $L^2(\Omega;d^nx)$ *and*

$$L^2(\Omega;d^nx)=\ker(H_{V,\max,\Omega})\oplus\big[(-\Delta+V)\,H_0^2(\Omega)\big], \tag{8.26}$$

as an orthogonal direct sum.

Our next theorem shows that there exists a countable family of orthonormal eigenfunctions for the perturbed Krein Laplacian which span the orthogonal complement of the kernel of this operator:

Theorem 8.4. *Assume Hypothesis* 6.2. *Then there exists a family of functions* $\{w_j\}_{j\in\mathbb{N}}$ *with the following properties:*

$$\begin{aligned} & w_j\in\operatorname{dom}(H_{K,\Omega})\cap H^{1/2}(\Omega)\ \text{ and}\\ & H_{K,\Omega}w_j=\lambda_{K,\Omega,j}w_j,\ \ \lambda_{K,\Omega,j}>0,\ j\in\mathbb{N}, \end{aligned} \tag{8.27}$$

$$(w_j,w_k)_{L^2(\Omega;d^nx)}=\delta_{j,k},\ j,k\in\mathbb{N}, \tag{8.28}$$

$$L^2(\Omega;d^nx)=\ker(H_{K,\Omega})\oplus\overline{\operatorname{lin.span}\{w_j\}_{j\in\mathbb{N}}}\ \ (\textit{orthogonal direct sum}). \tag{8.29}$$

Proof. That $w_j\in H^{1/2}(\Omega)$, $j\in\mathbb{N}$, follows from Proposition 7.3(i). The rest is a direct consequence of Lemma 8.3, the fact that

$$\ker(H_{V,\max,\Omega})=\big\{u\in L^2(\Omega;d^nx)\,\big|\,(-\Delta+V)u=0\big\}=\ker(H_{K,\Omega}), \tag{8.30}$$

the second part of Theorem 7.2, and Lemma 8.1 in which we set $w_j:=(-\Delta+V)u_j$, $j\in\mathbb{N}$. □

Next, we define the following Rayleigh quotient

$$R_{K,\Omega}[u]:=\frac{\|(-\Delta+V)u\|^2_{L^2(\Omega;d^nx)}}{\|\nabla u\|^2_{(L^2(\Omega;d^nx))^n}+\|V^{1/2}u\|^2_{L^2(\Omega;d^nx)}},\quad 0\neq u\in H_0^2(\Omega). \tag{8.31}$$

Then the following min-max principle holds:

Proposition 8.5. *Assume Hypothesis* 6.2. *Then*

$$\lambda_{K,\Omega,j}=\min_{\substack{W_j\ \text{subspace of}\ H_0^2(\Omega)\\ \dim(W_j)=j}}\Big(\max_{0\neq u\in W_j}R_{K,\Omega}[u]\Big),\quad j\in\mathbb{N}. \tag{8.32}$$

As a consequence, given two domains Ω, $\widetilde{\Omega}$ *as in Hypothesis* 5.7 *for which* $\Omega\subseteq\widetilde{\Omega}$, *and given a potential* $0\leq\widetilde{V}\in L^\infty(\widetilde{\Omega})$, *one has*

$$0<\widetilde{\lambda}_{K,\widetilde{\Omega},j}\leq\lambda_{K,\Omega,j},\quad j\in\mathbb{N}, \tag{8.33}$$

where $V:=\widetilde{V}|_\Omega$, *and* $\lambda_{K,\Omega,j}$ *and* $\widetilde{\lambda}_{K,\widetilde{\Omega},j}$, $j\in\mathbb{N}$, *are the eigenvalues corresponding to the Krein–von Neumann extensions associated with* Ω,V *and* $\widetilde{\Omega},\widetilde{V}$, *respectively.*

Proof. Obviously, (8.33) is a consequence of (8.32), so we will concentrate on the latter. We recall the Hilbert space $\mathcal{H}_V$ from (8.5) and the orthogonal family $\{u_j\}_{j\in\mathbb{N}}$ in (8.20)–(8.22). Next, consider the following subspaces of $\mathcal{H}_V$,

$$V_0 := \{0\}, \quad V_j := \operatorname{lin.span}\{u_i \,|\, 1 \le i \le j\}, \quad j \in \mathbb{N}. \tag{8.34}$$

Finally, set

$$V_j^{\perp} := \{u \in \mathcal{H} \,|\, [u, u_i]_{\mathcal{H}_V} = 0,\, 1 \le i \le j\}, \quad j \in \mathbb{N}. \tag{8.35}$$

We claim that

$$\lambda_{K,\Omega,j} = \min_{0 \ne u \in V_{j-1}^{\perp}} R_{K,\Omega}[u] = R_{K,\Omega}[u_j], \quad j \in \mathbb{N}. \tag{8.36}$$

Indeed, if $j \in \mathbb{N}$ and $u = \sum_{k=1}^{\infty} c_k u_k \in V_{j-1}^{\perp}$, then $c_k = 0$ whenever $1 \le k \le j-1$. Consequently,

$$\|(-\Delta + V)u\|^2_{L^2(\Omega;d^nx)} = \bigg\| \sum_{k=j}^{\infty} c_k(-\Delta + V)u_k \bigg\|^2_{L^2(\Omega;d^nx)} = \sum_{k=j}^{\infty} |c_k|^2 \tag{8.37}$$

by (8.3), so that

$$\begin{aligned}
\|\nabla u\|^2_{(L^2(\Omega;d^nx))^n} &+ \|V^{1/2}u\|^2_{L^2(\Omega;d^nx)} = ((-\Delta + V)u, u)_{L^2(\Omega;d^nx)} \\
&= \bigg(\sum_{k=j}^{\infty} c_k(-\Delta + V)u_k, u \bigg)_{L^2(\Omega;d^nx)} \\
&= \bigg(\sum_{k=j}^{\infty} (\lambda_{K,\Omega,k})^{-1} c_k(-\Delta + V)^2 u_k, u \bigg)_{L^2(\Omega;d^nx)} \\
&= \bigg(\sum_{k=j}^{\infty} (\lambda_{K,\Omega,k})^{-1} c_k(-\Delta + V)u_k, (-\Delta + V)u \bigg)_{L^2(\Omega;d^nx)} \\
&= \bigg(\sum_{k=j}^{\infty} (\lambda_{K,\Omega,k})^{-1} c_k(-\Delta + V)u_k, \sum_{k=j}^{\infty} c_k(-\Delta + V)u_k \bigg)_{L^2(\Omega;d^nx)} \\
&= \sum_{k=j}^{\infty} (\lambda_{K,\Omega,k})^{-1} |c_k|^2 \le (\lambda_{K,\Omega,j})^{-1} \sum_{k=j}^{\infty} |c_k|^2 \\
&= (\lambda_{K,\Omega,j})^{-1} \|(-\Delta + V)u\|^2_{L^2(\Omega;d^nx)},
\end{aligned} \tag{8.38}$$

where in the third step we have relied on (8.2), and the last step is based on (8.37). Thus, $R_{K,\Omega}[u] \ge \lambda_{K,\Omega,j}$ with equality if $u = u_j$ (cf. the calculation leading up to (7.4)). This proves (8.36). In fact, the same type of argument as the one just performed also shows that

$$\lambda_{K,\Omega,j} = \max_{0 \ne u \in V_j} R_{K,\Omega}[u] = R_{K,\Omega}[u_j], \quad j \in \mathbb{N}. \tag{8.39}$$

Next, we claim that if W_j is an arbitrary subspace of $\mathcal{H}$ of dimension j then

$$\lambda_{K,\Omega,j} \le \max_{0 \ne u \in W_j} R_{K,\Omega}[u], \quad j \in \mathbb{N}. \tag{8.40}$$

To justify this inequality, observe that $W_j \cap V_{j-1}^{\perp} \neq \{0\}$ by dimensional considerations. Hence, if $0 \neq v_j \in W_j \cap V_{j-1}^{\perp}$ then

$$\lambda_{K,\Omega,j} = \min_{0 \neq u \in V_{j-1}^{\perp}} R_{K,\Omega}[u] \leq R_{K,\Omega}[v_j] \leq \max_{0 \neq u \in W_j} R_{K,\Omega}[u], \tag{8.41}$$

establishing (8.40). Now formula (8.32) readily follows from this and (8.39). □

If $\Omega \subset \mathbb{R}^n$ is a bounded Lipschitz domain denote by

$$0 < \lambda_{D,\Omega,1} \leq \lambda_{D,\Omega,2} \leq \cdots \leq \lambda_{D,\Omega,j} \leq \lambda_{D,\Omega,j+1} \leq \cdots \tag{8.42}$$

the collection of eigenvalues for the perturbed Dirichlet Laplacian $H_{D,\Omega}$ (again, listed according to their multiplicity). Then, if $0 \leq V \in L^\infty(\Omega; d^n x)$, we have the well-known formula (cf., e.g., [64] for the case where $V \equiv 0$)

$$\lambda_{D,\Omega,j} = \min_{\substack{W_j \text{ subspace of } H_0^1(\Omega) \\ \dim(W_j)=j}} \Big(\max_{0 \neq u \in W_j} R_{D,\Omega}[u] \Big), \quad j \in \mathbb{N}, \tag{8.43}$$

where $R_{D,\Omega}[u]$, the Rayleigh quotient for the perturbed Dirichlet Laplacian, is given by

$$R_{D,\Omega}[u] := \frac{\|\nabla u\|^2_{(L^2(\Omega;d^n x))^n} + \|V^{1/2} u\|^2_{L^2(\Omega;d^n x)}}{\|u\|^2_{L^2(\Omega;d^n x)}}, \quad 0 \neq u \in H_0^1(\Omega). \tag{8.44}$$

From Theorem 2.10, Theorem 4.8, and Proposition 5.10, we already know that, granted Hypothesis 6.2, the nonzero eigenvalues of the perturbed Krein Laplacian are at least as large as the corresponding eigenvalues of the perturbed Dirichlet Laplacian. It is nonetheless of interest to provide a direct, analytical proof of this result. We do so in the proposition below.

Proposition 8.6. *Assume Hypothesis* 6.2. *Then*

$$0 < \lambda_{D,\Omega,j} \leq \lambda_{K,\Omega,j}, \quad j \in \mathbb{N}. \tag{8.45}$$

Proof. By the density of $C_0^\infty(\Omega)$ into $H_0^2(\Omega)$ and $H_0^1(\Omega)$, respectively, we obtain from (8.32) and (8.43) that

$$\lambda_{K,\Omega,j} = \inf_{\substack{W_j \text{ subspace of } C_0^\infty(\Omega) \\ \dim(W_j)=j}} \Big(\sup_{0 \neq u \in W_j} R_{K,\Omega}[u] \Big), \tag{8.46}$$

$$\lambda_{D,\Omega,j} = \inf_{\substack{W_j \text{ subspace of } C_0^\infty(\Omega) \\ \dim(W_j)=j}} \Big(\sup_{0 \neq u \in W_j} R_{D,\Omega}[u] \Big), \tag{8.47}$$

for every $j \in \mathbb{N}$. Since, if $u \in C_0^\infty(\Omega)$,

$$\begin{aligned} \|\nabla u\|^2_{(L^2(\Omega;d^n x))^n} + \|V^{1/2} u\|^2_{L^2(\Omega;d^n x)} &= ((-\Delta + V)u, u)_{L^2(\Omega;d^n x)} \\ &\leq \|(-\Delta + V)u\|_{L^2(\Omega;d^n x)} \|u\|_{L^2(\Omega;d^n x)}, \end{aligned} \tag{8.48}$$

we deduce that

$$R_{D,\Omega}[u] \leq R_{K,\Omega}[u], \text{ whenever } 0 \neq u \in C_0^\infty(\Omega). \tag{8.49}$$

With this at hand, (8.45) follows from (8.46)–(8.47). □

Remark 8.7. Another analytical approach to (8.45) which highlights the connection between the perturbed Krein Laplacian and a fourth-order boundary problem is as follows. Granted Hypotheses 4.1 and 4.7, and given $\lambda \in \mathbb{C}$, consider the following eigenvalue problem

$$\begin{cases} u \in \operatorname{dom}(-\Delta_{\max,\Omega}), \quad (-\Delta + V)u \in \operatorname{dom}(-\Delta_{\max,\Omega}), \\ (-\Delta + V)^2 u = \lambda\,(-\Delta + V)u \text{ in } \Omega, \\ \widehat{\gamma}_D(u) = 0 \text{ in } \Big(N^{1/2}(\partial\Omega)\Big)^*, \\ \widehat{\gamma}_D((-\Delta + V)u) = 0 \text{ in } \Big(N^{1/2}(\partial\Omega)\Big)^*. \end{cases} \tag{8.50}$$

Associated with it is the sesquilinear form

$$\begin{cases} \widetilde{a}_{V,\lambda}(\,\cdot\,,\,\cdot\,) : \widetilde{\mathcal{H}} \times \widetilde{\mathcal{H}} \longrightarrow \mathbb{C}, \quad \widetilde{\mathcal{H}} := H^2(\Omega) \cap H_0^1(\Omega), \\ \widetilde{a}_{V,\lambda}(u,v) := ((-\Delta + V)u, (-\Delta + V)v)_{L^2(\Omega;d^nx)} + \big(V^{1/2}u, V^{1/2}v\big)_{L^2(\Omega;d^nx)} \\ \qquad\qquad -\lambda\,(\nabla u, \nabla v)_{(L^2(\Omega;d^nx))^n}, \quad u, v \in \widetilde{\mathcal{H}}, \end{cases} \tag{8.51}$$

which has the property that

$$u \in \widetilde{\mathcal{H}} \text{ satisfies } \widetilde{a}_{V,\lambda}(u,v) = 0 \text{ for every } v \in \widetilde{\mathcal{H}} \text{ if and only if } u \text{ solves (8.50).} \tag{8.52}$$

We note that since the operator $-\Delta + V : H^2(\Omega) \cap H_0^1(\Omega) \to L^2(\Omega; d^n x)$ is an isomorphism, it follows that $u \mapsto \|(-\Delta + V)u\|_{L^2(\Omega;d^nx)}$ is an equivalent norm on the Banach space $\widetilde{\mathcal{H}}$, and the form $\widetilde{a}_{V,\lambda}(\,\cdot\,,\,\cdot\,)$ is coercive if $\lambda < -M$, where $M = M(\Omega, V) > 0$ is a sufficiently large constant. Based on this and proceeding as in Section 7, it can then be shown that the problem (8.50) has nontrivial solutions if and only if λ belongs to an exceptional set $\widetilde{\Lambda}_{\Omega,V} \subset (0, \infty)$ which is discrete and only accumulates at infinity. Furthermore, u solves (8.50) if and only if $v := (-\Delta + V)u$ is an eigenfunction for $H_{D,\Omega}$, corresponding to the eigenvalue λ and, conversely, if u is an eigenfunction for $H_{D,\Omega}$ corresponding to the eigenvalue λ, then u solves (8.50). Consequently, the problem (8.50) is spectrally equivalent to $H_{D,\Omega}$. From this, it follows that the eigenvalues $\{\lambda_{D,\Omega,j}\}_{j\in\mathbb{N}}$ of $H_{D,\Omega}$ can be expressed as

$$\lambda_{D,\Omega,j} = \min_{\substack{W_j \text{ subspace of } \widetilde{\mathcal{H}} \\ \dim(W_j)=j}} \Big(\max_{0 \neq u \in W_j} R_{K,\Omega}[u] \Big), \quad j \in \mathbb{N}, \tag{8.53}$$

where the Rayleigh quotient $R_{K,\Omega}[u]$ is as in (8.31). The upshot of this representation is that it immediately yields (8.45), on account of (8.32) and the fact that $H_0^2(\Omega) \subset \widetilde{\mathcal{H}}$.

Next, let Ω be as in Hypothesis 4.1 and $0 \leq V \in L^\infty(\Omega; d^n x)$. For $\lambda \in \mathbb{R}$ set

$$N_{X,\Omega}(\lambda) := \#\{j \in \mathbb{N} \,|\, \lambda_{X,\Omega,j} \leq \lambda\}, \quad X \in \{D, K\}, \tag{8.54}$$

where $\#S$ denotes the cardinality of the set S.

Corollary 8.8. *Assume Hypothesis* 6.2. *Then*

$$N_{K,\Omega}(\lambda) \leq N_{D,\Omega}(\lambda), \quad \lambda \in \mathbb{R}. \tag{8.55}$$

In particular,

$$N_{K,\Omega}(\lambda) = O(\lambda^{n/2}) \ \text{ as } \ \lambda \to \infty. \tag{8.56}$$

Proof. Estimate (8.55) is a trivial consequence of (8.45), whereas (8.56) follows from (8.42) and Weyl's asymptotic formula for the Dirichlet Laplacian in a Lipschitz domain (cf. [40] and the references therein for very general results of this nature). ☐

8.2. The unperturbed case

What we have proved in Section 7 and Section 8.1 shows that all known eigenvalue estimates for the (standard) buckling problem

$$u \in H_0^2(\Omega), \quad \Delta^2 u = -\lambda\, \Delta u \ \text{ in } \ \Omega, \tag{8.57}$$

valid in the class of domains described in Hypothesis 5.7, automatically hold, in the same format, for the Krein Laplacian (corresponding to $V \equiv 0$). For example, we have the following result with $\lambda^{(0)}_{K,\Omega,j}$, $j \in \mathbb{N}$, denoting the nonzero eigenvalues of the Krein Laplacian $-\Delta_{K,\Omega}$ and $\lambda^{(0)}_{D,\Omega,j}$, $j \in \mathbb{N}$, denoting the eigenvalues of the Dirichlet Laplacian $-\Delta_{D,\Omega}$:

Theorem 8.9. *If $\Omega \subset \mathbb{R}^n$ is as in Hypothesis* 5.7, *the nonzero eigenvalues of the Krein Laplacian $-\Delta_{K,\Omega}$ satisfy*

$$\lambda^{(0)}_{K,\Omega,2} \leq \frac{n^2+8n+20}{(n+2)^2}\lambda^{(0)}_{K,\Omega,1}, \tag{8.58}$$

$$\sum_{j=1}^{n} \lambda^{(0)}_{K,\Omega,j+1} < (n+4)\lambda^{(0)}_{K,\Omega,1} - \frac{4}{n+4}(\lambda^{(0)}_{K,\Omega,2} - \lambda^{(0)}_{K,\Omega,1}) \leqslant (n+4)\lambda^{(0)}_{K,\Omega,1}, \tag{8.59}$$

$$\sum_{j=1}^{k} \big(\lambda^{(0)}_{K,\Omega,k+1} - \lambda^{(0)}_{K,\Omega,j}\big)^2 \leq \frac{4(n+2)}{n^2} \sum_{j=1}^{k} \big(\lambda^{(0)}_{K,\Omega,k+1} - \lambda_{K,0,j}\big)\lambda^{(0)}_{K,\Omega,j}, \quad k \in \mathbb{N}, \tag{8.60}$$

Furthermore, if $j_{(n-2)/2,1}$ is the first positive zero of the Bessel function of first kind and order $(n-2)/2$ (cf. [1, Sect. 9.5]*), v_n denotes the volume of the unit ball in $\mathbb{R}^n$, and $|\Omega|$ stands for the n-dimensional Euclidean volume of Ω, then*

$$\frac{2^{2/n} j^2_{(n-2)/2,1} v_n^{2/n}}{|\Omega|^{2/n}} < \lambda^{(0)}_{D,\Omega,2} \leq \lambda^{(0)}_{K,\Omega,1}. \tag{8.61}$$

Proof. With the eigenvalues of the buckling plate problem replacing the corresponding eigenvalues of the Krein Laplacian, estimates (8.58)–(8.60) have been proved in [26], [27], [28], [60], and [110] (indeed, further strengthenings of (8.59) are detailed in [27], [28]), whereas the respective parts of (8.61) are covered by results in [122] and [150] (see also [31], [47]). □

Remark 8.10. Given the physical interpretation of the first eigenvalue for (8.57), it follows that $\lambda^{(0)}_{K,\Omega,1}$, the first nonzero eigenvalue for the Krein Laplacian $-\Delta_{K,\Omega}$, is proportional to the load compression at which the plate Ω (assumed to be as in Hypothesis 5.7) buckles. In this connection, it is worth remembering the long-standing conjecture of Pólya–Szegő, to the effect that amongst all plates of a given area, the circular one will buckle first (assuming all relevant physical parameters to be identical). In [31], the authors have given a partial result in this direction which, in terms of the first eigenvalue $\lambda^{(0)}_{K,\Omega,1}$ for the Krein Laplacian $-\Delta_{K,\Omega}$ in a domain Ω as in Hypothesis 5.7, reads

$$\lambda^{(0)}_{K,\Omega,1} > \frac{2^{2/n} j^2_{(n-2)/2,1} v_n^{2/n}}{|\Omega|^{2/n}} = c_n \lambda^{(0)}_{K,\Omega^\#,1} \tag{8.62}$$

where $\Omega^\#$ is the n-dimensional ball with the same volume as Ω, and

$$c_n = 2^{2/n}[j_{(n-2)/2,1}/j_{n/2,1}]^2 = 1 - (4 - \log 4)/n + O(n^{-5/3}) \to 1 \text{ as } n \to \infty. \tag{8.63}$$

This result implies an earlier inequality of Bramble and Payne [47] for the two-dimensional case, which reads

$$\lambda^{(0)}_{K,\Omega,1} > \frac{2\pi j^2_{0,1}}{\text{Area}\,(\Omega)}. \tag{8.64}$$

Given that (8.58) states a universal inequality for the ratio of the first two nonzero eigenvalues of the Krein Laplacian, that is, of the buckling problem, it is natural to wonder what the best upper bound for this ratio might be, and the shape of domain that saturates it. While this question is still open, the conjecture that springs most naturally to mind is that the ratio is maximized by the disk/ball, and that in n dimensions the best upper bound is therefore $j^2_{(n+2)/2,1}/j^2_{n/2,1}$ (a ratio of squares of first positive zeros of Bessel functions of appropriate order). In the context of the buckling problem this conjecture was stated in [26] (see p. 129). This circle of ideas goes back to Payne, Pólya, and Weinberger [154, 155], who first considered bounds for ratios of eigenvalues and who formulated the corresponding conjecture for the first two membrane eigenvalues (i.e., that the disk/ball maximizes the ratio of the first two eigenvalues).

Before stating an interesting universal inequality concerning the ratio of the first (nonzero) Dirichlet and Krein Laplacian eigenvalues for a bounded domain with boundary of nonnegative Gaussian mean curvature (which includes, obviously, the case of a bounded convex domain), we recall a well-known result due to

Babuška and Výborný [34] concerning domain continuity of Dirichlet eigenvalues (see also [55], [56], [62], [80], [171], [186], and the literature cited therein):

Theorem 8.11. *Let $\Omega \subset \mathbb{R}^n$ be open and bounded, and suppose that $\Omega_m \subset \Omega$, $m \in \mathbb{N}$, are open and monotone increasing toward Ω, that is,*

$$\Omega_m \subset \Omega_{m+1} \subset \Omega, \ m \in \mathbb{N}, \quad \bigcup_{m\in\mathbb{N}} \Omega_m = \Omega. \tag{8.65}$$

In addition, let $-\Delta_{D,\Omega_m}$ and $-\Delta_{D,\Omega}$ be the Dirichlet Laplacians in $L^2(\Omega_m; d^n x)$ and $L^2(\Omega; d^n x)$ (cf. (4.47), (4.53)), and denote their respective spectra by

$$\sigma(-\Delta_{D,\Omega_m}) = \big\{\lambda^{(0)}_{D,\Omega_m,j}\big\}_{j\in\mathbb{N}}, \ m \in \mathbb{N}, \ \text{ and } \sigma(-\Delta_{D,\Omega}) = \big\{\lambda^{(0)}_{D,\Omega,j}\big\}_{j\in\mathbb{N}}. \tag{8.66}$$

Then, for each $j \in \mathbb{N}$,

$$\lim_{m\to\infty} \lambda^{(0)}_{D,\Omega_m,j} = \lambda^{(0)}_{D,\Omega,j}. \tag{8.67}$$

Theorem 8.12. *Assume that $\Omega \subset \mathbb{R}^n$ is a bounded quasi-convex domain. In addition, assume there exists a sequence of C^∞-smooth domains $\{\Omega_m\}_{m\in\mathbb{N}}$ satisfying the following two conditions:*

(i) *The sequence $\{\Omega_m\}_{m\in\mathbb{N}}$ monotonically converges to Ω from inside, that is,*

$$\Omega_m \subset \Omega_{m+1} \subset \Omega, \ m \in \mathbb{N}, \quad \bigcup_{m\in\mathbb{N}} \Omega_m = \Omega. \tag{8.68}$$

(ii) *If $\mathcal{G}_m$ denotes the Gaussian mean curvature of $\partial\Omega_m$, then*

$$\mathcal{G}_m \geq 0 \ \text{ for all } m \in \mathbb{N}. \tag{8.69}$$

Then the first Dirichlet eigenvalue and the first nonzero eigenvalue for the Krein Laplacian in Ω satisfy

$$1 \leq \frac{\lambda^{(0)}_{K,\Omega,1}}{\lambda^{(0)}_{D,\Omega,1}} \leq 4. \tag{8.70}$$

In particular, each bounded convex domain $\Omega \subset \mathbb{R}^n$ satisfies conditions (i) *and* (ii) *and hence* (8.70) *holds for such domains.*

Proof. Of course, the lower bound in (8.70) is contained in (8.45), so we will concentrate on establishing the upper bound. To this end, we recall that it is possible to approximate Ω with a sequence of C^∞-smooth bounded domains satisfying (8.68) and (8.69). By Theorem 8.11, the Dirichlet eigenvalues are continuous under the domain perturbations described in (8.68) and one obtains, in particular,

$$\lim_{m\to\infty} \lambda^{(0)}_{D,\Omega_m,1} = \lambda^{(0)}_{D,\Omega,1}. \tag{8.71}$$

On the other hand, (8.33) yields that $\lambda^{(0)}_{K,\Omega,1} \leq \lambda^{(0)}_{K,\Omega_m,1}$. Together with (8.71), this shows that it suffices to prove that

$$\lambda^{(0)}_{K,\Omega_m,1} \leq 4\lambda^{(0)}_{D,\Omega_m,1}, \quad m \in \mathbb{N}. \tag{8.72}$$

Summarizing, it suffices to show that

$$\begin{gathered}\Omega \subset \mathbb{R}^n \text{ a bounded, } C^\infty\text{-smooth domain, whose Gaussian mean} \\ \text{curvature } \mathcal{G} \text{ of } \partial\Omega \text{ is nonnegative, implies } \lambda^{(0)}_{K,\Omega,1} \leq 4\,\lambda^{(0)}_{D,\Omega,1}.\end{gathered} \tag{8.73}$$

Thus, we fix a bounded, C^∞ domain $\Omega \subset \mathbb{R}^n$ with $\mathcal{G} \geq 0$ on $\partial\Omega$ and denote by u_1 the (unique, up to normalization) first eigenfunction for the Dirichlet Laplacian in Ω. In the sequel, we abbreviate $\lambda_D := \lambda^{(0)}_{D,\Omega,1}$ and $\lambda_K := \lambda^{(0)}_{K,\Omega,1}$. Then (cf. [92, Theorems 8.13 and 8.38]),

$$u_1 \in C^\infty(\overline{\Omega}), \quad u_1|_{\partial\Omega} = 0, \quad u_1 > 0 \text{ in } \Omega, \quad -\Delta u_1 = \lambda_D\, u_1 \text{ in } \Omega, \tag{8.74}$$

and

$$\lambda_D = \frac{\int_\Omega d^n x\, |\nabla u_1|^2}{\int_\Omega d^n x\, |u_1|^2}. \tag{8.75}$$

In addition, (8.36) (with $j = 1$) and u_1^2 as a "trial function" yields

$$\lambda_K \leq \frac{\int_\Omega d^n x\, |\Delta(u_1^2)|^2}{\int_\Omega d^n x\, |\nabla(u_1^2)|^2}. \tag{8.76}$$

Then (8.73) follows as soon as one shows that the right-hand side of (8.76) is less than or equal to the quadruple of the right-hand side of (8.75). For bounded, smooth, convex domains in the plane (i.e., for $n = 2$), such an estimate was established in [151]. For the convenience of the reader, below we review Payne's ingenious proof, primarily to make sure that it continues to hold in much the same format for our more general class of domains and in all space dimensions (in the process, we also shed more light on some less explicit steps in Payne's original proof, including the realization that the key hypothesis is not convexity of the domain, but rather nonnegativity of the Gaussian mean curvature $\mathcal{G}$ of its boundary). To get started, we expand

$$(\Delta(u_1^2))^2 = 4\big[\lambda_D^2 u_1^4 - 2\lambda_D\, u_1^2 |\nabla u_1|^2 + |\nabla u_1|^4\big], \quad |\nabla(u_1^2)|^2 = 4\, u_1^2 |\nabla u_1|^2, \tag{8.77}$$

and use (8.76) to write

$$\lambda_K \leq \lambda_D^2 \left(\frac{\int_\Omega d^n x\, u_1^4}{\int_\Omega d^n x\, u_1^2 |\nabla u_1|^2} \right) - 2\lambda_D + \left(\frac{\int_\Omega d^n x\, |\nabla u_1|^4}{\int_\Omega d^n x\, u_1^2 |\nabla u_1|^2} \right). \tag{8.78}$$

Next, observe that based on (8.74) and the Divergence Theorem we may write

$$\begin{aligned}\int_\Omega d^n x\, \big[3u_1^2 |\nabla u_1|^2 - \lambda_D\, u_1^4\big] &= \int_\Omega d^n x\, \big[3u_1^2 |\nabla u_1|^2 + u_1^3 \Delta u_1\big] = \int_\Omega d^n x\, \operatorname{div}\big(u_1^3 \nabla u_1\big) \\ &= \int_{\partial\Omega} d^{n-1}\omega\, u_1^3 \partial_\nu u_1 = 0,\end{aligned} \tag{8.79}$$

where ν is the outward unit normal to $\partial\Omega$, and $d^{n-1}\omega$ denotes the induced surface measure on $\partial\Omega$. This shows that the coefficient of λ_D^2 in (8.78) is $3\lambda_D^{-1}$, so that

$$\lambda_K \leq \lambda_D + \theta, \ \text{ where } \theta := \frac{\int_\Omega d^n x\, |\nabla u_1|^4}{\int_\Omega d^n x\, u_1^2 |\nabla u_1|^2}. \tag{8.80}$$

We begin to estimate θ by writing

$$\int_\Omega d^n x\, |\nabla u_1|^4 = \int_\Omega d^n x\, (\nabla u_1)\cdot(|\nabla u_1|^2 \nabla u_1) = -\int_\Omega d^n x\, u_1\, \mathrm{div}(|\nabla u_1|^2\nabla u_1)$$
$$= -\int_\Omega d^n x\, \big[(u_1\, \nabla u_1)\cdot(\nabla|\nabla u_1|^2) - \lambda_D\, u_1^2|\nabla u_1|^2\big], \tag{8.81}$$

so that

$$\frac{\int_\Omega d^n x\, (u_1\,\nabla u_1)\cdot(\nabla|\nabla u_1|^2)}{\int_\Omega d^n x\, u_1^2|\nabla u_1|^2} = \lambda_D - \theta. \tag{8.82}$$

To continue, one observes that because of (8.74) and the classical Hopf lemma (cf. [92, Lemma 3.4]) one has $\partial_\nu u_1 < 0$ on $\partial\Omega$. Thus, $|\nabla u_1| \neq 0$ at points in Ω near $\partial\Omega$. This allows one to conclude that

$$\nu = -\frac{\nabla u_1}{|\nabla u_1|} \text{ near and on } \partial\Omega. \tag{8.83}$$

By a standard result from differential geometry (see, for example, [69, p. 142])

$$\mathrm{div}(\nu) = (n-1)\,\mathcal{G} \text{ on } \partial\Omega, \tag{8.84}$$

where $\mathcal{G}$ denotes the mean curvature of $\partial\Omega$.

To proceed further, we introduce the following notations for the second derivative matrix, or *Hessian*, of u_1 and its norm:

$$\mathrm{Hess}(u_1) := \left(\frac{\partial^2 u_1}{\partial x_j \partial x_k}\right)_{1\le j,k\le n}, \quad |\mathrm{Hess}(u_1)| := \left(\sum_{j,k=1}^n |\partial_j\partial_k u_1|^2\right)^{1/2}. \tag{8.85}$$

Relatively brief and straightforward computations (cf. [123, Theorem 2.2.14]) then yield

$$\mathrm{div}(\nu) = -\sum_{j=1}^n \partial_j\left(\frac{\partial_j u_1}{|\nabla u_1|}\right) = |\nabla u_1|^{-1}[-\Delta u_1 + \langle \nu, \mathrm{Hess}(u_1)\nu\rangle]$$
$$= |\nabla u_1|^{-1}\langle \nu, \mathrm{Hess}(u_1)\nu\rangle \text{ on } \partial\Omega \tag{8.86}$$

(since $-\Delta u_1 = \lambda_D u_1 = 0$ on $\partial\Omega$),

$$\nu\cdot(\partial_\nu \nu) = -\sum_{j,k=1}^n \nu_j\nu_k\partial_k\left(\frac{\partial_j u_1}{|\nabla u_1|}\right) \tag{8.87}$$
$$= -|\nabla u_1|^{-1}\langle \nu, \mathrm{Hess}(u_1)\nu\rangle + |\nabla u_1|^{-1}|\nu|^2\langle \nu, \mathrm{Hess}(u_1)\nu\rangle = 0,$$

and finally, by (8.86),

$$\partial_\nu(|\nabla u_1|^2) = \sum_{j,k=1}^n \nu_j\partial_j[(\partial_k u_1)^2] = 2\sum_{j,k=1}^n \nu_j(\partial_k u_1)(\partial_j\partial_k u_1)$$
$$= -2|\nabla u_1|\langle \nu, \mathrm{Hess}(u_1)\nu\rangle = -2|\nabla u_1|^2\mathrm{div}(\nu)$$
$$= -2(n-1)\mathcal{G}|\nabla u_1|^2 \le 0 \text{ on } \partial\Omega, \tag{8.88}$$

given our assumption $\mathcal{G} \ge 0$.

Next, we compute

$$\begin{aligned}
&\int_\Omega d^n x\, \big[|\nabla(|\nabla u_1|^2)|^2 - 2\lambda_D\, |\nabla u_1|^4 + 2|\nabla u_1|^2 |\mathrm{Hess}(u_1)|^2\big] \\
&\quad = \int_\Omega d^n x\, div\big(|\nabla u_1|^2 \nabla(|\nabla u_1|^2)\big) = \int_{\partial\Omega} d^{n-1}\omega\, \nu \cdot \big(|\nabla u_1|^2 \nabla(|\nabla u_1|^2)\big) \\
&\quad = \int_{\partial\Omega} d^{n-1}\omega\, |\nabla u_1|^2 \partial_\nu\big(|\nabla u_1|^2\big) \leq 0,
\end{aligned} \tag{8.89}$$

since $\partial_\nu(|\nabla u_1|^2) \leq 0$ on $\partial\Omega$ by (8.88). As a consequence,

$$2\lambda_D \int_\Omega d^n x\, |\nabla u_1|^4 \geq \int_\Omega d^n x\, \big[|\nabla(|\nabla u_1|^2)|^2 + 2|\nabla u_1|^2 |\mathrm{Hess}(u_1)|^2\big]. \tag{8.90}$$

Now, simple algebra shows that $|\nabla(|\nabla u_1|^2)|^2 \leq 4\, |\nabla u_1|^2 |\mathrm{Hess}(u_1)|^2$ which, when combined with (8.90), yields

$$\frac{4\lambda_D}{3} \int_\Omega d^n x\, |\nabla u_1|^4 \geq \int_\Omega d^n x\, |\nabla(|\nabla u_1|^2)|^2. \tag{8.91}$$

Let us now return to (8.81) and rewrite this equality as

$$\int_\Omega d^n x\, |\nabla u_1|^4 = -\int_\Omega d^n x\, (u_1 \nabla u_1) \cdot (\nabla |\nabla u_1|^2 - \lambda_D\, u_1 \nabla u_1). \tag{8.92}$$

An application of the Cauchy–Schwarz inequality then yields

$$\left(\int_\Omega d^n x\, |\nabla u_1|^4\right)^2 \leq \left(\int_\Omega d^n x\, u_1^2\, |\nabla u_1|^2\right) \left(\int_\Omega d^n x\, |\nabla |\nabla u_1|^2 - \lambda_D\, u_1 \nabla u_1|^2\right). \tag{8.93}$$

By expanding the last integrand and recalling the definition of θ we then arrive at

$$\theta^2 \leq \lambda_D^2 - 2\lambda_D \left(\frac{\int_\Omega d^n x\, (u_1 \nabla u_1) \cdot (\nabla |\nabla u_1|^2)}{\int_\Omega d^n x\, u_1^2 |\nabla u_1|^2}\right) + \left(\frac{\int_\Omega d^n x\, |\nabla(|\nabla u_1|^2)|^2}{\int_\Omega d^n x\, u_1^2 |\nabla u_1|^2}\right). \tag{8.94}$$

Upon recalling (8.82) and (8.91), this becomes

$$\theta^2 \leq \lambda_D^2 - 2\lambda_D(\lambda_D - \theta) + \frac{4\lambda_D}{3}\theta = -\lambda_D^2 + \frac{10\lambda_D}{3}\theta. \tag{8.95}$$

In turn, this forces $\theta \leq 3\lambda_D$ hence, ultimately, $\lambda_K \leq 4\lambda_D$ due to this estimate and (8.80). This establishes (8.73) and completes the proof of the theorem. □

Remark 8.13. (i) The upper bound in (8.70) for two-dimensional smooth, convex C^∞ domains Ω is due to Payne [151] in 1960. He notes that the proof carries over without difficulty to dimensions $n \geq 2$ in [152, p. 464]. In addition, one can avoid assuming smoothness in his proof by using smooth approximations Ω_m, $m \in \mathbb{N}$, of Ω as discussed in our proof. Of course, Payne did not consider the eigenvalues of the Krein Laplacian $-\Delta_{K,\Omega}$, instead, he compared the first eigenvalue of the fixed membrane problem and the first eigenvalue of the problem of the buckling of a clamped plate.

(ii) By thinking of Hess(u_1) represented in terms of an orthonormal basis for $\mathbb{R}^n$ that contains ν, one sees that (8.86) yields

$$\operatorname{div}(\nu) = \left|\frac{\partial u_1}{\partial \nu}\right|^{-1} \frac{\partial^2 u_1}{\partial \nu^2} = -\left(\frac{\partial u_1}{\partial \nu}\right)^{-1} \frac{\partial^2 u_1}{\partial \nu^2} \tag{8.96}$$

(the latter because $\partial u_1/\partial\nu < 0$ on $\partial\Omega$ by our convention on the sign of u_1 (see (8.74))), and thus

$$\frac{\partial^2 u_1}{\partial \nu^2} = -(n-1)\mathcal{G}\frac{\partial u_1}{\partial \nu} \text{ on } \partial\Omega. \tag{8.97}$$

For a different but related argument leading to this same result, see Ashbaugh and Levine [32, pp. I-8, I-9]. Aviles [33], Payne [150], [151], and Levine and Weinberger [132] all use similar arguments as well.

(iii) We note that Payne's basic result here, when done in n dimensions, holds for smooth domains having a boundary which is everywhere of nonnegative mean curvature. In addition, Levine and Weinberger [132], in the context of a related problem, consider nonsmooth domains for the nonnegative mean curvature case and a variety of cases intermediate between that and the convex case (including the convex case).

(iv) Payne's argument (and the constant 4 in Theorem 8.12) would appear to be sharp, with any infinite slab in $\mathbb{R}^n$ bounded by parallel hyperplanes being a saturating case (in a limiting sense). We note that such a slab is essentially one-dimensional, and that, up to normalization, the first Dirichlet eigenfunction u_1 for the interval $[0, a]$ (with $a > 0$) is

$$u_1(x) = \sin(\pi x/a) \text{ with eigenvalue } \lambda = \pi^2/a^2, \tag{8.98}$$

while the corresponding first buckling eigenfunction and eigenvalue are

$$u_1(x)^2 = \sin^2(\pi x/a) = [1 - \cos(2\pi x/a)]/2 \text{ and } 4\lambda = 4\pi^2/a^2. \tag{8.99}$$

Thus, Payne's choice of the trial function u_1^2, where u_1 is the first Dirichlet eigenfunction should be optimal for this limiting case, implying that the bound 4 is best possible. Payne, too, made observations about the equality case of his inequality, and observed that the infinite strip saturates it in 2 dimensions. His supporting arguments are via tracing the case of equality through the inequalities in his proof, which also yields interesting insights.

Remark 8.14. The eigenvalues corresponding to the buckling of a two-dimensional *square* plate, clamped along its boundary, have been analyzed numerically by several authors (see, e.g., [8], [9], and [46]). All these results can now be naturally reinterpreted in the context of the Krein Laplacian $-\Delta_{K,\Omega}$ in the case where $\Omega = (0,1)^2 \subset \mathbb{R}^2$. Lower bounds for the first k buckling problem eigenvalues were discussed in [131]. The existence of convex domains Ω, for which the first eigenfunction of the problem of a clamped plate and the problem of the buckling of a clamped plate possesses a change of sign, was established in [121]. Relations between an eigenvalue problem governing the behavior of an elastic medium and the buckling problem were studied in [111]. Buckling eigenvalues as a function of the elasticity constant are investigated in [115]. Finally, spectral properties of linear operator pencils $A - \lambda B$ with discrete spectra, and basis properties of the corresponding eigenvectors, applicable to differential operators, were discussed, for instance, in [156], [175] (see also the references cited therein).

Formula (8.56) suggests the issue of deriving a Weyl asymptotic formula for the perturbed Krein Laplacian $H_{K,\Omega}$. This is the topic of our next section.

9. Weyl asymptotics for the perturbed Krein Laplacian in nonsmooth domains

We begin by recording a very useful result due to V.A. Kozlov which, for the convenience of the reader, we state here in more generality than is actually required for our purposes. To set the stage, let $\Omega \subset \mathbb{R}^n$, $n \geqslant 2$, be a bounded Lipschitz domain. In addition, assume that $m > r \geq 0$ are two fixed integers and set

$$\eta := 2(m-r) > 0. \tag{9.1}$$

Let W be a closed subspace in $H^m(\Omega)$ such that $H_0^m(\Omega) \subseteq W$. On W, consider the symmetric forms

$$a(u,v) := \sum_{0\leq|\alpha|,|\beta|\leq m} \int_\Omega d^n x\, a_{\alpha,\beta}(x)\overline{(\partial^\beta u)(x)}(\partial^\alpha v)(x), \quad u,v \in W, \tag{9.2}$$

and

$$b(u,v) := \sum_{0\leq|\alpha|,|\beta|\leqslant r} \int_\Omega d^n x\, b_{\alpha,\beta}(x)\overline{(\partial^\beta u)(x)}(\partial^\alpha v)(x), \quad u,v \in W. \tag{9.3}$$

Suppose that the leading coefficients in $a(\,\cdot\,,\,\cdot\,)$ and $b(\,\cdot\,,\,\cdot\,)$ are Lipschitz functions, while the coefficients of all lower-order terms are bounded, measurable functions in Ω. Furthermore, assume that the following coercivity, nondegeneracy, and nonnegativity conditions hold: For some $C_0 \in (0,\infty)$,

$$a(u,u) \geqslant C_0\|u\|^2_{H^m(\Omega)}, \quad u \in W, \tag{9.4}$$

$$\sum_{|\alpha|=|\beta|=r} b_{\alpha,\beta}(x)\,\xi^{\alpha+\beta} \neq 0, \quad x \in \overline{\Omega},\ \xi \neq 0, \tag{9.5}$$

$$b(u,u) \geqslant 0, \quad u \in W. \tag{9.6}$$

Under the above assumptions, W can be regarded as a Hilbert space when equipped with the inner product $a(\,\cdot\,,\,\cdot\,)$. Next, consider the operator $T \in \mathcal{B}(W)$ uniquely defined by the requirement that

$$a(u,Tv) = b(u,v), \quad u,v \in W. \tag{9.7}$$

Then the operator T is compact, nonnegative and self-adjoint on W (when the latter is viewed as a Hilbert space). Going further, denote by

$$0 \leq \cdots \leq \mu_{j+1}(T) \leq \mu_j(T) \leq \cdots \leq \mu_1(T), \tag{9.8}$$

the eigenvalues of T listed according to their multiplicity, and set

$$N(\lambda; W, a, b) := \#\{j \in \mathbb{N} \,|\, \mu_j(T) \geq \lambda^{-1}\}, \quad \lambda > 0. \tag{9.9}$$

The following Weyl asymptotic formula is a particular case of a slightly more general result which can be found in [119].

Theorem 9.1. *Assume Hypothesis* 4.1 *and retain the above notation and assumptions on* $a(\,\cdot\,,\,\cdot\,)$, $b(\,\cdot\,,\,\cdot\,)$, W, *and* T. *In addition, we recall* (9.1). *Then the distribution function of the spectrum of* T *introduced in* (9.9) *satisfies the asymptotic formula*

$$N(\lambda; W, a, b) = \omega_{a,b,\Omega}\, \lambda^{n/\eta} + O\big(\lambda^{(n-(1/2))/\eta}\big) \ \text{ as } \ \lambda \to \infty, \tag{9.10}$$

where, with $d\omega_{n-1}$ *denoting the surface measure on the unit sphere* $S^{n-1} = \{\xi \in \mathbb{R}^n \,|\, |\xi| = 1\}$ *in* $\mathbb{R}^n$,

$$\omega_{a,b,\Omega} := \frac{1}{n(2\pi)^n} \int_\Omega d^n x \left(\int_{|\xi|=1} d\omega_{n-1}(\xi) \left[\frac{\sum_{|\alpha|=|\beta|=r} b_{\alpha,\beta}(x)\xi^{\alpha+\beta}}{\sum_{|\alpha|=|\beta|=m} a_{\alpha,\beta}(x)\xi^{\alpha+\beta}} \right]^{\frac{n}{\eta}} \right). \tag{9.11}$$

Various related results can be found in [118], [120]. After this preamble, we are in a position to state and prove the main result of this section:

Theorem 9.2. *Assume Hypothesis* 6.2. *In addition, we recall that*

$$N_{K,\Omega}(\lambda) = \#\{j \in \mathbb{N} \,|\, \lambda_{K,\Omega,j} \leq \lambda\}, \quad \lambda \in \mathbb{R}, \tag{9.12}$$

where the (*strictly*) *positive eigenvalues* $\{\lambda_{K,\Omega,j}\}_{j\in\mathbb{N}}$ *of the perturbed Krein Laplacian* $H_{K,\Omega}$ *are enumerated as in* (8.1) (*according to their multiplicities*). *Then the following Weyl asymptotic formula holds:*

$$N_{K,\Omega}(\lambda) = (2\pi)^{-n} v_n |\Omega|\, \lambda^{n/2} + O\big(\lambda^{(n-(1/2))/2}\big) \ \text{ as } \ \lambda \to \infty, \tag{9.13}$$

where, as before, v_n *denotes the volume of the unit ball in* $\mathbb{R}^n$, *and* $|\Omega|$ *stands for the* n*-dimensional Euclidean volume of* Ω.

Proof. Set $W := H_0^2(\Omega)$ and consider the symmetric forms

$$a(u,v) := \int_\Omega d^n x\, \overline{(-\Delta + V)u}\, (-\Delta + V)v, \quad u, v \in W, \tag{9.14}$$

$$b(u,v) := \int_\Omega d^n x\, \overline{\nabla u} \cdot \nabla v + \int_\Omega d^n x\, \overline{V^{1/2} u}\, V^{1/2} v, \quad u, v \in W, \tag{9.15}$$

for which conditions (9.4)–(9.6) (with $m = 2$) are verified (cf. (8.6)). Next, we recall the operator $(-\Delta + V)^{-2} := ((-\Delta + V)^2)^{-1} \in \mathcal{B}\big(H^{-2}(\Omega), H_0^2(\Omega)\big)$ from (8.11) along with the operator

$$B \in \mathcal{B}_\infty(W), \quad Bu := -(-\Delta + V)^{-2}(-\Delta + V)u, \quad u \in W, \tag{9.16}$$

from (8.13). Then, in the current notation, formula (8.15) reads $a(Bu, v) = b(u, v)$ for every $u, v \in C_0^\infty(\Omega)$. Hence, by density,

$$a(Bu, v) = b(u, v), \quad u, v \in W. \tag{9.17}$$

This shows that actually $B = T$, the operator originally introduced in (9.7). In particular, T is one-to-one. Consequently, $Tu = \mu\, u$ for $u \in W$ and $0 \neq \mu \in \mathbb{C}$, if and only if $u \in H_0^2(\Omega)$ satisfies $(-\Delta+V)^{-2}(-\Delta+V)u = \mu\, u$, that is, $(-\Delta+V)^2 u = \mu^{-1}(-\Delta + V)u$. Hence, the eigenvalues of T are precisely the reciprocals of the eigenvalues of the buckling clamped plate problem (7.6). Having established this, formula (9.13) then follows from Theorem 7.5 and (9.10), upon observing that in our case $m = 2$, $r = 1$ (hence $\eta = 2$) and $\omega_{a,b,\Omega} = (2\pi)^{-n} v_n |\Omega|$. □

Incidentally, Theorem 9.2 and Theorem 7.5 show that, granted Hypothesis 6.2, a Weyl asymptotic formula holds in the case of the (perturbed) buckling problem (7.1). For smoother domains and potentials, this is covered by Grubb's results in [97]. In the smooth context, a sharpening of the remainder has been derived in [143], [144], and most recently, in [102].

In the case where $\Omega \subset \mathbb{R}^2$ is a bounded domain with a C^∞-boundary and $0 \leq V \in C^\infty(\overline{\Omega})$, a more precise form of the error term in (9.13) was obtained in [97] where Grubb has shown that

$$N_{K,\Omega}(\lambda) = \frac{|\Omega|}{4\pi}\,\lambda + O\big(\lambda^{2/3}\big) \text{ as } \lambda \to \infty, \tag{9.18}$$

In fact, in [97], Grubb deals with the Weyl asymptotic for the Krein–von Neumann extension of a general strongly elliptic, formally self-adjoint differential operator of arbitrary order, provided both its coefficients as well as the underlying domain $\Omega \subset \mathbb{R}^n$ $(n \geq 2)$ are C^∞-smooth. In the special case where Ω equals the open ball $B_n(0; R)$, $R > 0$, in $\mathbb{R}^n$, and when $V \equiv 0$, it turns out that (9.13), (9.18) can be further refined to

$$\begin{aligned} N^{(0)}_{K,B_n(0;R)}(\lambda) &= (2\pi)^{-n} v_n^2 R^n \lambda^{n/2} - (2\pi)^{-(n-1)} v_{n-1}[(n/4)v_n + v_{n-1}]R^{n-1}\lambda^{(n-1)/2} \\ &\quad + O\big(\lambda^{(n-2)/2}\big) \text{ as } \lambda \to \infty, \end{aligned} \tag{9.19}$$

for every $n \geq 2$. This will be the object of the final Section 11 (cf. Proposition 11.1).

10. A class of domains for which the Krein and Dirichlet Laplacians coincide

Motivated by the special example where $\Omega = \mathbb{R}^2\backslash\{0\}$ and $S = \overline{-\Delta_{C_0^\infty(\mathbb{R}^2\backslash\{0\})}}$, in which case one can show the interesting fact that $S_F = S_K$ (cf. [12], [13, Ch. I.5], [83], and Subsections 11.4 and 11.5) and hence the nonnegative self-adjoint extension of S is unique, the aim of this section is to present a class of (nonempty, proper) open sets $\Omega = \mathbb{R}^n\backslash K$, $K \subset \mathbb{R}^n$ compact and subject to a vanishing Bessel capacity condition, with the property that the Friedrichs and Krein–von Neumann extensions of $-\Delta\big|_{C_0^\infty(\Omega)}$ in $L^2(\Omega; d^n x)$, coincide. To the best of our knowledge, the case where the set K differs from a single point is without precedent and so the following results for more general sets K appear to be new.

We start by making some definitions and discussing some preliminary results, of independent interest. Given an arbitrary open set $\Omega \subset \mathbb{R}^n$, $n \geq 2$, we consider three realizations of $-\Delta$ as unbounded operators in $L^2(\Omega; d^n x)$, with domains given by (cf. Subsection 4.2)

$$\mathrm{dom}(-\Delta_{\max,\Omega}) := \big\{u \in L^2(\Omega; d^n x) \,\big|\, \Delta u \in L^2(\Omega; d^n x)\big\}, \tag{10.1}$$

$$\mathrm{dom}(-\Delta_{D,\Omega}) := \big\{u \in H_0^1(\Omega) \,\big|\, \Delta u \in L^2(\Omega; d^n x)\big\}, \tag{10.2}$$

$$\mathrm{dom}(-\Delta_{c,\Omega}) := C_0^\infty(\Omega). \tag{10.3}$$

Lemma 10.1. *For any open, nonempty subset $\Omega \subseteq \mathbb{R}^n$, $n \geq 2$, the following statements hold:*

(i) *One has*

$$(-\Delta_{c,\Omega})^* = -\Delta_{\max,\Omega}. \tag{10.4}$$

(ii) *The Friedrichs extension of $-\Delta_{c,\Omega}$ is given by*

$$(-\Delta_{c,\Omega})_F = -\Delta_{D,\Omega}. \tag{10.5}$$

(iii) *The Krein–von Neumann extension of $-\Delta_{c,\Omega}$ has the domain*

$$\mathrm{dom}((-\Delta_{c,\Omega})_K) = \big\{u \in \mathrm{dom}(-\Delta_{\max,\Omega}) \,\big|\, \text{there exists } \{u_j\}_{j\in\mathbb{N}} \in C_0^\infty(\Omega) \tag{10.6}$$
$$\text{with } \lim_{j\to\infty} \|\Delta u_j - \Delta u\|_{L^2(\Omega; d^n x)} = 0 \text{ and } \{\nabla u_j\}_{j\in\mathbb{N}} \text{ Cauchy in } L^2(\Omega; d^n x)^n\big\}.$$

(iv) *One has*

$$\ker((-\Delta_{c,\Omega})_K) = \big\{u \in L^2(\Omega; d^n x) \,\big|\, \Delta u = 0 \text{ in } \Omega\big\}, \tag{10.7}$$

and

$$\ker((-\Delta_{c,\Omega})_F) = \{0\}. \tag{10.8}$$

Proof. Formula (10.4) follows in a straightforward fashion, by unravelling definitions, whereas (10.5) is a direct consequence of (2.14) or (2.19) (compare also with Proposition 5.10). Next, (10.6) is readily implied by (2.20) and (10.4). In addition, (10.7) is easily derived from (2.12), (10.4) and (10.1). Finally, consider (10.8). In a first stage, (10.5) and (10.2) yield that

$$\ker((-\Delta_{c,\Omega})_F) = \big\{u \in H_0^1(\Omega) \,\big|\, \Delta u = 0 \text{ in } \Omega\big\}, \tag{10.9}$$

so the goal is to show that the latter space is trivial. To this end, pick a function $u \in H_0^1(\Omega)$ which is harmonic in Ω, and observe that this forces $\nabla u = 0$ in Ω. Now, with tilde denoting the extension by zero outside Ω, we have $\widetilde{u} \in H^1(\mathbb{R}^n)$ and $\nabla(\widetilde{u}) = \widetilde{\nabla u}$. In turn, this entails that $\widetilde{u}$ is a constant function in $L^2(\mathbb{R}; d^n x)$ and hence $u \equiv 0$ in Ω, establishing (10.8). □

Next, we record some useful capacity results. For an authoritative extensive discussion on this topic see the monographs [3], [137], [174], and [191]. We denote by $B_{\alpha,2}(E)$ the Bessel capacity of order $\alpha > 0$ of a set $E \subset \mathbb{R}^n$. When $K \subset \mathbb{R}^n$ is a compact set, this is defined by

$$B_{\alpha,2}(K) := \inf\big\{\|f\|^2_{L^2(\mathbb{R}^n; d^n x)} \,\big|\, g_\alpha * f \geq 1 \text{ on } K,\ f \geq 0\big\}, \tag{10.10}$$

where the Bessel kernel g_α is defined as the function whose Fourier transform is given by

$$\widehat{g_\alpha}(\xi) = (2\pi)^{-n/2}(1+|\xi|^2)^{-\alpha/2}, \quad \xi \in \mathbb{R}^n. \tag{10.11}$$

When $\mathcal{O} \subseteq \mathbb{R}^n$ is open, we define

$$B_{\alpha,2}(\mathcal{O}) := \sup\{B_{\alpha,2}(K) \,|\, K \subset \mathcal{O},\, K \text{ compact}\}, \tag{10.12}$$

and, finally, when $E \subseteq \mathbb{R}^n$ is an arbitrary set,

$$B_{\alpha,2}(E) := \inf\{B_{\alpha,2}(\mathcal{O}) \,|\, \mathcal{O} \supset E,\, \mathcal{O} \text{ open}\}. \tag{10.13}$$

In addition, denote by $\mathcal{H}^k$ the k-dimensional Hausdorff measure on $\mathbb{R}^n$, $0 \leq k \leq n$. Finally, a compact subset $K \subset \mathbb{R}^n$ is said to be *L^2-removable for the Laplacian* provided every bounded, open neighborhood $\mathcal{O}$ of K has the property that

$$u \in L^2(\mathcal{O}\backslash K; d^n x) \text{ with } \Delta u = 0 \text{ in } \mathcal{O}\backslash K \text{ imply } \begin{cases} \text{there exists } \widetilde{u} \in L^2(\mathcal{O}; d^n x) \\ \text{so that } \widetilde{u}\big|_{\mathcal{O}\backslash K} = u \text{ and} \\ \Delta \widetilde{u} = 0 \text{ in } \mathcal{O}. \end{cases} \tag{10.14}$$

Proposition 10.2. *For $\alpha > 0$, $k \in \mathbb{N}$, $n \geq 2$ and $E \subset \mathbb{R}^n$, the following properties are valid:*

(i) *A compact set $K \subset \mathbb{R}^n$ is L^2-removable for the Laplacian if and only if $B_{2,2}(K) = 0$.*

(ii) *Assume that $\Omega \subset \mathbb{R}^n$ is an open set and that $K \subset \Omega$ is a closed set. Then the space $C_0^\infty(\Omega\backslash K)$ is dense in $H^k(\Omega)$ (i.e., one has the natural identification $H_0^k(\Omega) \equiv H_0^k(\Omega\backslash K)$), if and only if $B_{k,2}(K) = 0$.*

(iii) *If $2\alpha \leq n$ and $\mathcal{H}^{n-2\alpha}(E) < +\infty$ then $B_{\alpha,2}(E) = 0$. Conversely, if $2\alpha \leq n$ and $B_{\alpha,2}(E) = 0$ then $\mathcal{H}^{n-2\alpha+\varepsilon}(E) = 0$ for every $\varepsilon > 0$.*

(iv) *Whenever $2\alpha > n$ then there exists $C = C(\alpha, n) > 0$ such that $B_{\alpha,2}(E) \geq C$ provided $E \neq \emptyset$.*

See, [3, Corollary 3.3.4], [137, Theorem 3], [191, Theorem 2.6.16 and Remark 2.6.15], respectively. For other useful removability criteria the interested reader may wish to consult [59], [136], [162], and [177].

The first main result of this section is then the following:

Theorem 10.3. *Assume that $K \subset \mathbb{R}^n$, $n \geq 3$, is a compact set with the property that*

$$B_{2,2}(K) = 0. \tag{10.15}$$

Define $\Omega := \mathbb{R}^n\backslash K$. Then, in the domain Ω, the Friedrichs and Krein–von Neumann extensions of $-\Delta$, initially considered on $C_0^\infty(\Omega)$, coincide, that is,

$$(-\Delta_{c,\Omega})_F = (-\Delta_{c,\Omega})_K. \tag{10.16}$$

As a consequence, $-\Delta|_{C_0^\infty(\Omega)}$ has a unique nonnegative self-adjoint extension in $L^2(\Omega; d^n x)$.

Proof. We note that (10.15) implies that K has zero n-dimensional Lebesgue measure, so that $L^2(\Omega; d^n x) \equiv L^2(\mathbb{R}^n; d^n x)$. In addition, by *(iii)* in Proposition 10.2, we also have $B_{1,2}(K) = 0$. Now, if $u \in \mathrm{dom}(-\Delta_{c,\Omega})_K$, (10.6) entails that $u \in L^2(\Omega; d^n x)$, $\Delta u \in L^2(\Omega; d^n x)$, and that there exists a sequence $u_j \in C_0^\infty(\Omega)$, $j \in \mathbb{N}$, for which

$$\Delta u_j \to \Delta u \text{ in } L^2(\Omega; d^n x) \text{ as } j \to \infty, \text{ and } \{\nabla u_j\}_{j\in\mathbb{N}} \text{ is Cauchy in } L^2(\Omega; d^n x). \tag{10.17}$$

In view of the well-known estimate (cf. the Corollary on p. 56 of [137]),

$$\|v\|_{L^{2^*}(\mathbb{R}^n; d^n x)} \le C_n \|\nabla v\|_{L^2(\mathbb{R}^n; d^n x)}, \quad v \in C_0^\infty(\mathbb{R}^n), \tag{10.18}$$

where $2^* := (2n)/(n-2)$, the last condition in (10.17) implies that there exists $w \in L^{2^*}(\mathbb{R}^n; d^n x)$ with the property that

$$u_j \to w \text{ in } L^{2^*}(\mathbb{R}^n; d^n x) \text{ and } \nabla u_j \to \nabla w \text{ in } L^2(\mathbb{R}^n; d^n x) \text{ as } j \to \infty. \tag{10.19}$$

Furthermore, by the first convergence in (10.17), we also have that $\Delta w = \Delta u$ in the sense of distributions in Ω. In particular, the function

$$f := w - u \in L^{2^*}(\mathbb{R}^n; d^n x) + L^2(\mathbb{R}^n; d^n x) \hookrightarrow L^2_{\mathrm{loc}}(\mathbb{R}^n; d^n x) \tag{10.20}$$

satisfies $\Delta f = 0$ in $\Omega = \mathbb{R}^n \backslash K$. Granted (10.15), Proposition 10.2 yields that K is L^2-removable for the Laplacian, so we may conclude that $\Delta f = 0$ in $\mathbb{R}^n$. With this at hand, Liouville's theorem then ensures that $f \equiv 0$ in $\mathbb{R}^n$. This forces $u = w$ as distributions in Ω and hence, $\nabla u = \nabla w$ distributionally in Ω. In view of the last condition in (10.19) we may therefore conclude that $u \in H^1(\mathbb{R}^n) = H^1_0(\mathbb{R}^n)$. With this at hand, Proposition 10.2 yields that $u \in H^1_0(\Omega)$. This proves that $\mathrm{dom}(-\Delta_{c,\Omega})_K \subseteq \mathrm{dom}(-\Delta_{c,\Omega})_F$ and hence, $(-\Delta_{c,\Omega})_K \subseteq (-\Delta_{c,\Omega})_F$. Since both operators in question are self-adjoint, (10.16) follows. □

We emphasize that equality of the Friedrichs and Krein Laplacians necessarily requires that fact that $\inf(\sigma((-\Delta_{c,\Omega})_F)) = \inf(\sigma((-\Delta_{c,\Omega})_K)) = 0$, and hence rules out the case of bounded domains $\Omega \subset \mathbb{R}^n$, $n \in \mathbb{N}$ (for which $\inf(\sigma((-\Delta_{c,\Omega})_F)) > 0$).

Corollary 10.4. *Assume that $K \subset \mathbb{R}^n$, $n \ge 4$, is a compact set with finite $(n-4)$-dimensional Hausdorff measure, that is,*

$$\mathcal{H}^{n-4}(K) < +\infty. \tag{10.21}$$

Then, with $\Omega := \mathbb{R}^n \backslash K$, one has $(-\Delta_{c,\Omega})_F = (-\Delta_{c,\Omega})_K$, and hence, $-\Delta|_{C_0^\infty(\Omega)}$ has a unique nonnegative self-adjoint extension in $L^2(\Omega; d^n x)$.

Proof. This is a direct consequence of Proposition 10.2 and Theorem 10.3. □

In closing, we wish to remark that, as a trivial particular case of the above corollary, formula (10.16) holds for the punctured space

$$\Omega := \mathbb{R}^n \backslash \{0\}, \quad n \ge 4, \tag{10.22}$$

however, this fact is also clear from the well-known fact that $-\Delta|_{C_0^\infty(\mathbb{R}^n \backslash \{0\})}$ is essentially self-adjoint in $L^2(\mathbb{R}^n; d^n x)$ if (and only if) $n \ge 4$ (cf., e.g., [161, p. 161], and our discussion concerning the Bessel operator (11.118)). In [83, Example 4.9] (see also our discussion in Subsection 10.3), it has been shown (by using different methods) that (10.16) continues to hold for the choice (10.22) when $n = 2$, but that the Friedrichs and Krein–von Neumann extensions of $-\Delta$, initially considered on $C_0^\infty(\Omega)$ with Ω as in (10.22), are different when $n = 3$.

In light of Theorem 10.3, a natural question is whether the coincidence of the Friedrichs and Krein–von Neumann extensions of $-\Delta$, initially defined on $C_0^\infty(\Omega)$ for some open set $\Omega \subset \mathbb{R}^n$, actually implies that the complement of Ω has zero Bessel capacity of order two. Below, under some mild background assumptions on the domain in question, we shall establish this type of converse result. Specifically, we now prove the following fact:

Theorem 10.5. *Assume that $K \subset \mathbb{R}^n$, $n > 4$, is a compact set of zero n-dimensional Lebesgue measure, and set $\Omega := \mathbb{R}^n \backslash K$. Then*

$$(-\Delta_{c,\Omega})_F = (-\Delta_{c,\Omega})_K \ \text{ implies } \ B_{2,2}(K) = 0. \tag{10.23}$$

Proof. Let K be as in the statement of the theorem. In particular, $L^2(\Omega; d^n x) \equiv L^2(\mathbb{R}^n; d^n x)$. Hence, granted that $(-\Delta_{c,\Omega})_K = (-\Delta_{c,\Omega})_F$, in view of (10.7), (10.8) this yields

$$\big\{u \in L^2(\mathbb{R}^n; d^n x) \,\big|\, \Delta\, u = 0 \text{ in } \mathbb{R}^n \backslash K\big\} = \{0\}. \tag{10.24}$$

It is useful to think of (10.24) as a capacitary condition. More precisely, (10.24) implies that $\operatorname{Cap}(K) = 0$, where

$$\operatorname{Cap}(K) := \sup\big\{\big|{}_{\mathcal{E}'(\mathbb{R}^n)}\langle \Delta u, 1\rangle_{\mathcal{E}(\mathbb{R}^n)}\big| \,\big|\, \|u\|_{L^2(\mathbb{R}^n; d^n x)} \leq 1 \text{ and } \operatorname{supp}(\Delta u) \subseteq K\big\}. \tag{10.25}$$

Above, $\mathcal{E}(\mathbb{R}^n)$ is the space of smooth functions in $\mathbb{R}^n$ equipped with the usual Frechét topology, which ensures that its dual, $\mathcal{E}'(\mathbb{R}^n)$, is the space of compactly supported distributions in $\mathbb{R}^n$. At this stage, we recall the fundamental solution for the Laplacian in $\mathbb{R}^n$, $n \geq 3$, that is,

$$E_n(x) := \frac{\Gamma(n/2)}{2(2-n)\pi^{n/2}|x|^{n-2}}, \quad x \in \mathbb{R}^n \backslash \{0\} \tag{10.26}$$

($\Gamma(\cdot)$ the classical Gamma function [1, Sect. 6.1]), and introduce a related capacity, namely

$$\begin{aligned}\operatorname{Cap}_*(K) := \sup\big\{\big|{}_{\mathcal{E}'(\mathbb{R}^n)}\langle f, 1\rangle_{\mathcal{E}(\mathbb{R}^n)}\big| \,\big|\, & f \in \mathcal{E}'(\mathbb{R}^n), \\ & \operatorname{supp}(f) \subseteq K, \|E_n * f\|_{L^2(\mathbb{R}^n; d^n x)} \leq 1\big\}.\end{aligned} \tag{10.27}$$

Then

$$0 \leq \operatorname{Cap}_*(K) \leq \operatorname{Cap}(K) = 0 \tag{10.28}$$

so that $\operatorname{Cap}_*(K) = 0$. With this at hand, [104, Theorem 1.5 (a)] (here we make use of the fact that $n > 4$) then allows us to strengthen (10.24) to

$$\big\{u \in L^2_{\text{loc}}(\mathbb{R}^n; d^n x) \,\big|\, \Delta\, u = 0 \text{ in } \mathbb{R}^n \backslash K\big\} = \{0\}. \tag{10.29}$$

Next, we follow the argument used in the proof of [138, Lemma 5.5] and [3, Theorem 2.7.4]. Reasoning by contradiction, assume that $B_{2,2}(K) > 0$. Then there exists a nonzero, positive measure μ supported in K such that $g_2 * \mu \in L^2(\mathbb{R}^n)$. Since $g_2(x) = c_n\, E_n(x) + o(|x|^{2-n})$ as $|x| \to 0$ (cf. the discussion in Section 1.2.4 of [3]) this further implies that $E_n * \mu \in L^2_{\rm loc}(\mathbb{R}^n; d^n x)$. However, $E_n * \mu$ is a harmonic function in $\mathbb{R}^n \backslash K$, which is not identically zero since

$$\lim_{x\to\infty} |x|^{n-2}(E_n * \mu)(x) = c_n \mu(K) > 0, \tag{10.30}$$

so this contradicts (10.29). This shows that $B_{2,2}(K) = 0$. □

In this context we also refer to [82, Sect. 3.3] for necessary and sufficient conditions for equality of (certain generalizations of) the Friedrichs and the Krein Laplacians in terms of appropriate notions of capacity and Dirichlet forms.

Theorems 10.3–10.5 readily generalize to other types of elliptic operators (including higher-order systems). For example, using the polyharmonic operator $(-\Delta)^\ell$, $\ell \in \mathbb{N}$, as a prototype, we have the following result:

Theorem 10.6. *Fix $\ell \in \mathbb{N}$, $n \geq 2\ell + 1$, and assume that $K \subset \mathbb{R}^n$ is a compact set of zero n-dimensional Lebesgue measure. Define $\Omega := \mathbb{R}^n \backslash K$. Then, in the domain Ω, the Friedrichs and Krein–von Neumann extensions of the polyharmonic operator $(-\Delta)^\ell$, initially considered on $C_0^\infty(\Omega)$, coincide if and only if $B_{2\ell,2}(K) = 0$.*

For some related results in the punctured space $\Omega := \mathbb{R}^n \backslash \{0\}$, see also the recent article [4]. Moreover, we mention that in the case of the Bessel operator $h_\nu = (-d^2/dr^2) + (\nu^2 - (1/4))r^{-2}$ defined on $C_0^\infty((0,\infty))$, equality of the Friedrichs and Krein extension of h_ν in $L^2((0,\infty); dr)$ if and only if $\nu = 0$ has been established in [134]. (The sufficiency of the condition $\nu = 0$ was established earlier in [83].)

While this section focused on differential operators, we conclude with a very brief remark on half-line Jacobi, that is, tridiagonal (and hence, second-order finite difference) operators: As discussed in depth by Simon [169], the Friedrichs and Krein–von Neumann extensions of a minimally defined symmetric half-line Jacobi operator (cf. also [49]) coincide, if and only if the associated Stieltjes moment problem is determinate (i.e., has a unique solution) while the corresponding Hamburger moment problem is indeterminate (and hence has uncountably many solutions).

11. Examples

11.1. The case of a bounded interval (a,b), $-\infty < a < b < \infty$, $V = 0$

We briefly recall the essence of the one-dimensional example $\Omega = (a,b)$, $-\infty < a < b < \infty$, and $V = 0$. This was first discussed in detail by [14] and [81, Sect. 2.3] (see also [82, Sect. 3.3]).

Consider the minimal operator $-\Delta_{\min,(a,b)}$ in $L^2((a,b); dx)$, given by

$$\begin{aligned} & -\Delta_{\min,(a,b)} u = -u'', \\ & u \in \operatorname{dom}(-\Delta_{\min,(a,b)}) = \big\{ v \in L^2((a,b); dx) \,\big|\, v, v' \in AC([a,b]); \\ & \qquad v(a) = v'(a) = v(b) = v'(b) = 0;\ v'' \in L^2((a,b); dx) \big\}, \end{aligned} \tag{11.1}$$

where $AC([a,b])$ denotes the set of absolutely continuous functions on $[a,b]$. Evidently,

$$-\Delta_{\min,(a,b)} = \overline{-\frac{d^2}{dx^2}\bigg|_{C_0^\infty((a,b))}}, \tag{11.2}$$

and one can show that

$$-\Delta_{\min,(a,b)} \geq [\pi/(b-a)]^2 I_{L^2((a,b);dx)}. \tag{11.3}$$

In addition, one infers that

$$(-\Delta_{\min,(a,b)})^* = -\Delta_{\max,(a,b)}, \tag{11.4}$$

where

$$\begin{aligned} & -\Delta_{\max,(a,b)} u = -u'', \\ & u \in \operatorname{dom}(-\Delta_{\max,(a,b)}) = \big\{v \in L^2((a,b);dx) \,\big|\, v, v' \in AC([a,b]); \\ & \qquad\qquad v'' \in L^2((a,b);dx)\big\}. \end{aligned} \tag{11.5}$$

In particular,

$$\operatorname{def}(-\Delta_{\min,(a,b)}) = (2,2) \text{ and } \ker((-\Delta_{\min,(a,b)})^*) = \operatorname{lin.span}\{1, x\}. \tag{11.6}$$

The Friedrichs (equivalently, the Dirichlet) extension $-\Delta_{D,(a,b)}$ of $-\Delta_{\min,(a,b)}$ is then given by

$$\begin{aligned} & -\Delta_{D,(a,b)} u = -u'', \\ & u \in \operatorname{dom}(-\Delta_{D,(a,b)}) = \big\{v \in L^2((a,b);dx) \,\big|\, v, v' \in AC([a,b]); \\ & \qquad\qquad v(a) = v(b) = 0;\ v'' \in L^2((a,b);dx)\big\}. \end{aligned} \tag{11.7}$$

In addition,

$$\sigma(-\Delta_{D,(a,b)}) = \{j^2\pi^2(b-a)^{-2}\}_{j\in\mathbb{N}}, \tag{11.8}$$

and

$$\begin{aligned} \operatorname{dom}\big((-\Delta_{D,(a,b)})^{1/2}\big) = \big\{&v \in L^2((a,b);dx) \,\big|\, v \in AC([a,b]); \\ & v(a) = v(b) = 0;\ v' \in L^2((a,b);dx)\big\}. \end{aligned} \tag{11.9}$$

By (2.10),

$$\operatorname{dom}(-\Delta_{K,(a,b)}) = \operatorname{dom}(-\Delta_{\min,(a,b)}) \dotplus \ker((-\Delta_{\min,(a,b)})^*), \tag{11.10}$$

and hence any $u \in \operatorname{dom}(-\Delta_{K,(a,b)})$ is of the type

$$\begin{aligned} & u = f + \eta, \quad f \in \operatorname{dom}(-\Delta_{\min,(a,b)}), \\ & \eta(x) = u(a) + [u(b) - u(a)]\left(\frac{x-a}{b-a}\right),\ x \in (a,b), \end{aligned} \tag{11.11}$$

in particular, $f(a) = f'(a) = f(b) = f'(b) = 0$. Thus, the Krein–von Neumann extension $-\Delta_{K,(a,b)}$ of $-\Delta_{\min,(a,b)}$ is given by

$$\begin{aligned} & -\Delta_{K,(a,b)}u = -u'', \\ & u \in \operatorname{dom}(-\Delta_{K,(a,b)}) = \big\{v \in L^2((a,b);dx) \,\big|\, v, v' \in AC([a,b]); \\ & \qquad v'(a) = v'(b) = [v(b)-v(a)]/(b-a);\ v'' \in L^2((a,b);dx)\big\}. \end{aligned} \tag{11.12}$$

Using the characterization of all self-adjoint extensions of general Sturm–Liouville operators in [187, Theorem 13.14], one can also directly verify that $-\Delta_{K,(a,b)}$ as given by (11.12) is a self-adjoint extension of $-\Delta_{\min,(a,b)}$.

In connection with (11.1), (11.5), (11.7), and (11.12), we also note that the well-known fact that

$$v, v'' \in L^2((a,b);dx) \text{ implies } v' \in L^2((a,b);dx). \tag{11.13}$$

Utilizing (11.13), we briefly consider the quadratic form associated with the Krein Laplacian $-\Delta_{K,(a,b)}$. By (2.42) and (2.43), one infers,

$$\operatorname{dom}\big((-\Delta_{K,(a,b)})^{1/2}\big) = \operatorname{dom}\big((-\Delta_{D,(a,b)})^{1/2}\big) \dotplus \ker((-\Delta_{\min,(a,b)})^*), \tag{11.14}$$

$$\begin{aligned} & \big\|(-\Delta_{K,(a,b)})^{1/2}(u+g)\big\|^2_{L^2((a,b);dx)} = \big\|(-\Delta_{D,(a,b)})^{1/2}u\big\|^2_{L^2((a,b);dx)} \\ & \quad = ((u+g)', (u+g)')_{L^2((a,b);dx)} - [\overline{g(b)}g'(b) - \overline{g(a)}g'(a)] \\ & \quad = ((u+g)', (u+g)')_{L^2((a,b);dx)} - |[u(b)+g(b)] - [u(a)+g(a)]|^2/(b-a), \\ & \qquad\qquad u \in \operatorname{dom}\big((-\Delta_{D,(a,b)})^{1/2}\big),\ g \in \ker((-\Delta_{\min,(a,b)})^*). \end{aligned} \tag{11.15}$$

Finally, we turn to the spectrum of $-\Delta_{K,(a,b)}$. The boundary conditions in (11.12) lead to two kinds of (nonnormalized) eigenfunctions and eigenvalue equations

$$\begin{aligned} & \psi(k,x) = \cos(k(x - [(a+b)/2])), \quad k\sin(k(b-a)/2) = 0, \\ & k_{K,(a,b),j} = (j+1)\pi/(b-a),\ j = -1, 1, 3, 5, \dots, \end{aligned} \tag{11.16}$$

and

$$\begin{aligned} & \phi(k,x) = \sin(k(x - [(a+b)/2])), \quad k(b-a)/2 = \tan(k(b-a)/2), \\ & k_{K,(a,b),0} = 0,\ j\pi < k_{K,(a,b),j} < (j+1)\pi,\ j = 2, 4, 6, 8, \dots, \\ & \lim_{\ell\to\infty} [k_{K,(a,b),2\ell} - ((2\ell+1)\pi/(b-a))] = 0. \end{aligned} \tag{11.17}$$

The associated eigenvalues of $-\Delta_{K,(a,b)}$ are thus given by

$$\sigma(-\Delta_{K,(a,b)}) = \{0\} \cup \{k^2_{K,(a,b),j}\}_{j\in\mathbb{N}}, \tag{11.18}$$

where the eigenvalue 0 of $-\Delta_{K,(a,b)}$ is of multiplicity two, but the remaining nonzero eigenvalues of $-\Delta_{K,(a,b)}$ are all simple.

11.2. The case of a bounded interval (a,b), $-\infty < a < b < \infty$, $0 \leq V \in L^1((a,b);dx)$

The general case with a nonvanishing potential $0 \leq V \in L^1((a,b);dx)$ has very recently been worked out in [61]. We briefly summarize these findings next.

Suppose $\tau = -\frac{d^2}{dx^2} + V(x)$, $x \in (a,b)$, and $H_{\min,(a,b)}$, defined by

$$\begin{aligned} &H_{\min,(a,b)}u = -u'' + Vu, \\ &u \in \operatorname{dom}(H_{\min,(a,b)}) = \big\{v \in L^2((a,b);dx)\,\big|\, v,\, v' \in \mathrm{AC}([a,b]); \\ &\qquad\qquad v(a) = v'(a) = v(b) = v'(b) = 0; \\ &\qquad\qquad [-v'' + Vv] \in L^2((a,b);dx)\big\}, \end{aligned} \tag{11.19}$$

is strictly positive in the sense that there exists an $\varepsilon > 0$ for which

$$(u, H_{\min,(a,b)}u)_{L^2((a,b);dx)} \geq \varepsilon \|u\|^2_{L^2((a,b);dx)}, \quad u \in \operatorname{dom}(H_{\min,(a,b)}). \tag{11.20}$$

Since the deficiency indices of $H_{\min,(a,b)}$ are $(2,2)$, the assumption (11.20) implies that

$$\dim(\ker(H^*_{\min,(a,b)})) = 2. \tag{11.21}$$

As a basis for $\ker(H^*_{\min,(a,b)})$, we choose $\{u_1(\cdot), u_2(\cdot)\}$, where $u_1(\cdot)$ and $u_2(\cdot)$ are real valued and satisfy

$$u_1(a) = 0, \quad u_1(b) = 1, \quad u_2(a) = 1, \quad u_2(b) = 0. \tag{11.22}$$

The Krein–von Neumann extension $H_{K,(a,b)}$ of $H_{\min,(a,b)}$ in $L^2((a,b);dx)$ is defined as the restriction of $H^*_{\min,(a,b)}$ with domain

$$\operatorname{dom}(H_{K,(a,b)}) = \operatorname{dom}(H_{\min,(a,b)}) \dotplus \ker(H^*_{\min,(a,b)}). \tag{11.23}$$

Since $H_{K,(a,b)}$ is a self-adjoint extension of $H_{\min,(a,b)}$, functions in $\operatorname{dom}(H_{K,(a,b)})$ must satisfy certain boundary conditions; we now provide a characterization of these boundary conditions. Let $u \in \operatorname{dom}(H_{K,(a,b)})$; by (11.23) there exist $f \in \operatorname{dom}(H_{\min,(a,b)})$ and $\eta \in \ker(H^*_{\min,(a,b)})$ with

$$u(x) = f(x) + \eta(x), \quad x \in [a,b]. \tag{11.24}$$

Since $f \in \operatorname{dom}(H_{\min,(a,b)})$,

$$f(a) = f'(a) = f(b) = f'(b) = 0, \tag{11.25}$$

and as a result,

$$u(a) = \eta(a), \quad u(b) = \eta(b). \tag{11.26}$$

Since $\eta \in \ker(H^*_{\min,(a,b)})$, we write (cf. (11.22))

$$\eta(x) = c_1 u_1(0,x) + c_2 u_2(0,x), \quad x \in [a,b], \tag{11.27}$$

for appropriate scalars $c_1, c_2 \in \mathbb{C}$. By separately evaluating (11.27) at $x = a$ and $x = b$, one infers from (11.22) that

$$\eta(a) = c_2, \quad \eta(b) = c_1. \tag{11.28}$$

Comparing (11.28) and (11.26) allows one to write (11.27) as

$$\eta(x) = u(b)u_1(x) + u(a)u_2(x), \quad x \in [a,b]. \tag{11.29}$$

Finally, (11.24) and (11.29) imply

$$u(x) = f(x) + u(b)u_1(x) + u(a)u_2(x), \quad x \in [a,b], \tag{11.30}$$

and as a result,

$$u'(x) = f'(x) + u(b)u_1'(x) + u(a)u_2'(x), \quad x \in [a,b]. \tag{11.31}$$

Evaluating (11.31) separately at $x = a$ and $x = b$, and using (11.25) yields the following boundary conditions for u:

$$u'(a) = u(b)u_1'(a) + u(a)u_2'(a), \quad u'(b) = u(b)u_1'(b) + u(a)u_2'(b). \tag{11.32}$$

Since $u_1'(a) \neq 0$ (one recalls that $u_1(a) = 0$), relations (11.32) can be recast as

$$\begin{pmatrix} u(b) \\ u'(b) \end{pmatrix} = F_{\mathrm{K}} \begin{pmatrix} u(a) \\ u'(a) \end{pmatrix}, \tag{11.33}$$

where

$$F_{\mathrm{K}} = \frac{1}{u_1'(a)} \begin{pmatrix} -u_2'(a) & 1 \\ u_1'(a)u_2'(b) - u_1'(b)u_2'(a) & u_1'(b) \end{pmatrix}. \tag{11.34}$$

Then $F_{\mathrm{K}} \in \mathrm{SL}_2(\mathbb{R})$ since (11.34) implies

$$\det(F_{\mathrm{K}}) = -\frac{u_2'(b)}{u_1'(a)} = 1. \tag{11.35}$$

Thus, $H_{\mathrm{K},(a,b)}$, the Krein–von Neumann extension of $H_{\min,(a,b)}$ explicitly reads

$$\begin{aligned} &H_{\mathrm{K},(a,b)}u = -u'' + Vu, \\ &u \in \mathrm{dom}(H_{\mathrm{K},(a,b)}) = \bigg\{ v \in L^2((a,b);dx) \,\bigg|\, v,\, v' \in \mathrm{AC}([a,b]); \\ &\qquad \begin{pmatrix} v(b) \\ v'(b) \end{pmatrix} = F_{\mathrm{K}} \begin{pmatrix} v(a) \\ v'(a) \end{pmatrix};\ [-v'' + Vv] \in L^2((a,b);dx) \bigg\}. \end{aligned} \tag{11.36}$$

Taking $V \equiv 0$, one readily verifies that (11.36) reduces to (11.12) as in this case, a basis for $\ker(H^*_{\min,(a,b)})$ is provided by

$$u_1^{(0)}(x) = \frac{x-a}{b-a}, \quad u_2^{(0)}(x) = \frac{b-x}{b-a}, \quad x \in [a,b]. \tag{11.37}$$

The case $V \equiv 0$ and $-d^2/dx^2$ replaced by $-(d/dx)p(d/x)$, with $p > 0$ a.e., $p \in L^1_{\mathrm{loc}}((a,b);dx)$, $p^{-1} \in L^1((a,b);dx)$, was recently discussed in [76].

11.3. The case of the ball $B_n(0;R)$, $R>0$, in $\mathbb{R}^n$, $n\geq 2$, $V=0$

In this subsection, we consider in great detail the scenario when the domain Ω equals a ball of radius $R>0$ (for convenience, centered at the origin) in $\mathbb{R}^n$,

$$\Omega = B_n(0;R) \subset \mathbb{R}^n, \quad R>0,\ n\geqslant 2. \tag{11.38}$$

Since both the domain $B_n(0;R)$ in (11.38), as well as the Laplacian $-\Delta$ are invariant under rotations in $\mathbb{R}^n$ centered at the origin, we will employ the (angular momentum) decomposition of $L^2(B_n(0;R);d^nx)$ into the direct sum of tensor products

$$\begin{aligned} L^2(B_n(0;R);d^nx) &= L^2((0,R);r^{n-1}dr)\otimes L^2(S^{n-1};d\omega_{n-1}) \\ &= \bigoplus_{\ell\in\mathbb{N}_0} \mathcal{H}_{n,\ell,(0,R)}, \end{aligned} \tag{11.39}$$

$$\mathcal{H}_{n,\ell,(0,R)} = L^2((0,R);r^{n-1}dr)\otimes \mathcal{K}_{n,\ell}, \quad \ell\in\mathbb{N}_0,\ n\geq 2, \tag{11.40}$$

where $S^{n-1}=\partial B_n(0;1)=\{x\in\mathbb{R}^n \,|\, |x|=1\}$ denotes the $(n-1)$-dimensional unit sphere in $\mathbb{R}^n$, $d\omega_{n-1}$ represents the surface measure on S^{n-1}, $n\geq 2$, and $\mathcal{K}_{n,\ell}$ denoting the eigenspace of the Laplace–Beltrami operator $-\Delta_{S^{n-1}}$ in $L^2(S^{n-1};d\omega_{n-1})$ corresponding to the ℓth eigenvalue $\kappa_{n,\ell}$ of $-\Delta_{S^{n-1}}$ counting multiplicity,

$$\begin{aligned} &\kappa_{n,\ell} = \ell(\ell+n-2), \\ &\dim(\mathcal{K}_{n,\ell}) = \frac{(2\ell+n-2)\Gamma(\ell+n-2)}{\Gamma(\ell+1)\Gamma(n-1)} := d_{n,\ell}, \quad \ell\in\mathbb{N}_0,\ n\geq 2 \end{aligned} \tag{11.41}$$

(cf. [147, p. 4]). In other words, $\mathcal{K}_{n,\ell}$ is spanned by the n-dimensional spherical harmonics of degree $\ell\in\mathbb{N}_0$. For more details in this connection we refer to [161, App. to Sect. X.1] and [187, Ch. 18].

As a result, the minimal Laplacian in $L^2(B_n(0;R);d^nx)$ can be decomposed as follows

$$\begin{aligned} &-\Delta_{\min,B_n(0;R)} = \overline{-\Delta|_{C_0^\infty(B_n(0;R))}} = \bigoplus_{\ell\in\mathbb{N}_0} H^{(0)}_{n,\ell,\min}\otimes I_{\mathcal{K}_{n,\ell}}, \\ &\operatorname{dom}(-\Delta_{\min,B_n(0;R)}) = H_0^2(B_n(0;R)), \end{aligned} \tag{11.42}$$

where $H^{(0)}_{n,\ell,\min}$ in $L^2((0,R);r^{n-1}dr)$ are given by

$$H^{(0)}_{n,\ell,\min} = \overline{\left(-\frac{d^2}{dr^2}-\frac{n-1}{r}\frac{d}{dr}+\frac{\kappa_{n,\ell}}{r^2}\right)\Big|_{C_0^\infty((0,R))}}, \quad \ell\in\mathbb{N}_0. \tag{11.43}$$

Using the unitary operator U_n defined by

$$U_n\colon \begin{cases} L^2((0,R);r^{n-1}dr)\to L^2((0,R);dr), \\ \qquad\qquad \phi\mapsto (U_n\phi)(r) = r^{(n-1)/2}\phi(r), \end{cases} \tag{11.44}$$

it will also be convenient to consider the unitary transformation of $H^{(0)}_{n,\ell,\min}$ given by

$$h^{(0)}_{n,\ell,\min} = U_n H^{(0)}_{n,\ell,\min} U_n^{-1}, \quad \ell \in \mathbb{N}_0, \tag{11.45}$$

where

$$\begin{aligned} & h^{(0)}_{n,0,\min} = -\frac{d^2}{dr^2} + \frac{(n-1)(n-3)}{4r^2}, \quad 0<r<R, \\ & \operatorname{dom}\big(h^{(0)}_{n,0,\min}\big) = \big\{f \in L^2((0,R);dr) \,\big|\, f,f' \in AC([\varepsilon,R]) \text{ for all } \varepsilon>0; \\ & \qquad f(R_-) = f'(R_-) = 0,\ f_0 = 0; \\ & \qquad (-f'' + [(n-1)(n-3)/4]r^{-2}f) \in L^2((0,R);dr)\big\} \\ & \qquad \text{for } n=2,3, \end{aligned} \tag{11.46}$$

$$\begin{aligned} & h^{(0)}_{n,\ell,\min} = -\frac{d^2}{dr^2} + \frac{4\kappa_{n,\ell} + (n-1)(n-3)}{4r^2}, \quad 0<r<R, \\ & \operatorname{dom}\big(h^{(0)}_{n,\ell,\min}\big) = \big\{f \in L^2((0,R);dr) \,|\, f,f' \in AC([\varepsilon,R]) \ \text{ for all } \varepsilon>0; \\ & \qquad f(R_-) = f'(R_-) = 0; \\ & \qquad (-f'' + [\kappa_{n,\ell} + ((n-1)(n-3)/4)]r^{-2}f) \in L^2((0,R);dr)\big\} \\ & \qquad \text{for } \ell \in \mathbb{N},\ n \geq 2 \text{ and } \ell=0,\ n\geq 4. \end{aligned} \tag{11.47}$$

In particular, for $\ell \in \mathbb{N}$, $n \geq 2$, and $\ell = 0$, $n \geq 4$, one obtains

$$\begin{aligned} h^{(0)}_{n,\ell,\min} = \overline{\left(-\frac{d^2}{dr^2} + \frac{4\kappa_{n,\ell} + (n-1)(n-3)}{4r^2}\right)\bigg|_{C_0^\infty((0,R))}} \\ \text{for } \ell \in \mathbb{N},\ n\geq 2, \text{ and } \ell=0,\ n\geq 4. \end{aligned} \tag{11.48}$$

On the other hand, for $n = 2,3$, the domain of the closure of $h^{(0)}_{n,0,\min}\big|_{C_0^\infty((0,R))}$ is strictly contained in that of $\operatorname{dom}\big(h^{(0)}_{n,0,\min}\big)$, and in this case one obtains for

$$\widehat{h}^{(0)}_{n,0,\min} = \overline{\left(-\frac{d^2}{dr^2} + \frac{(n-1)(n-3)}{4r^2}\right)\bigg|_{C_0^\infty((0,R))}}, \quad n=2,3, \tag{11.49}$$

that

$$\begin{aligned} & \widehat{h}^{(0)}_{n,0,\min} = -\frac{d^2}{dr^2} + \frac{(n-1)(n-3)}{4r^2}, \quad 0<r<R, \\ & \operatorname{dom}\big(\widehat{h}^{(0)}_{n,0,\min}\big) = \big\{f \in L^2((0,R);dr) \,\big|\, f,f' \in AC([\varepsilon,R]) \text{ for all } \varepsilon>0; \\ & \qquad f(R_-) = f'(R_-) = 0,\ f_0 = f'_0 = 0; \\ & \qquad (-f'' + [(n-1)(n-3)/4]r^{-2}f) \in L^2((0,R);dr)\big\}. \end{aligned} \tag{11.50}$$

Here we used the abbreviations (cf. [54] for details)

$$f_0 = \begin{cases} \lim_{r\downarrow 0}[-r^{1/2}\ln(r)]^{-1}f(r), & n=2, \\ f(0_+), & n=3, \end{cases}$$
$$f_0' = \begin{cases} \lim_{r\downarrow 0} r^{-1/2}[f(r)+f_0 r^{1/2}\ln(r)], & n=2, \\ f'(0_+), & n=3. \end{cases} \tag{11.51}$$

We also recall the adjoints of $h^{(0)}_{n,\ell,\min}$ which are given by

$$\begin{aligned} &\big(h^{(0)}_{n,0,\min}\big)^* = -\frac{d^2}{dr^2} + \frac{(n-1)(n-3)}{4r^2}, \quad 0<r<R, \\ &\operatorname{dom}\big(\big(h^{(0)}_{n,0,\min}\big)^*\big) = \big\{f \in L^2((0,R);dr) \,\big|\, f,f' \in AC([\varepsilon,R]) \text{ for all } \varepsilon>0; \\ &\quad f_0 = 0;\ (-f'' + [(n-1)(n-3)/4]r^{-2}f) \in L^2((0,R);dr)\big\} \text{ for } n=2,3, \end{aligned} \tag{11.52}$$

$$\begin{aligned} &\big(h^{(0)}_{n,\ell,\min}\big)^* = -\frac{d^2}{dr^2} + \frac{4\kappa_{n,\ell} + (n-1)(n-3)}{4r^2}, \quad 0<r<R, \\ &\operatorname{dom}\big(\big(h^{(0)}_{n,\ell,\min}\big)^*\big) = \big\{f \in L^2((0,R);dr) \,\big|\, f,f' \in AC([\varepsilon,R]) \text{ for all } \varepsilon>0; \\ &\quad (-f'' + [\kappa_{n,\ell} + ((n-1)(n-3)/4)]r^{-2}f) \in L^2((0,R);dr)\big\} \\ &\quad \text{for } \ell\in\mathbb{N},\ n\geq 2 \text{ and } \ell=0,\ n\geq 4. \end{aligned} \tag{11.53}$$

In particular,

$$h^{(0)}_{n,\ell,max} = \big(h^{(0)}_{n,\ell,\min}\big)^*, \quad \ell\in\mathbb{N}_0,\ n\geq 2. \tag{11.54}$$

All self-adjoint extensions of $h^{(0)}_{n,\ell,\min}$ are given by the following one-parameter families $h^{(0)}_{n,\ell,\alpha_{n,\ell}}$, $\alpha_{n,\ell}\in\mathbb{R}\cup\{\infty\}$,

$$\begin{aligned} &h^{(0)}_{n,0,\alpha_{n,0}} = -\frac{d^2}{dr^2} + \frac{(n-1)(n-3)}{4r^2}, \quad 0<r<R, \\ &\operatorname{dom}\big(h^{(0)}_{n,0,\alpha_{n,0}}\big) = \big\{f \in L^2((0,R);dr) \,\big|\, f,f' \in AC([\varepsilon,R]) \text{ for all } \varepsilon>0; \\ &\quad f'(R_-) + \alpha_{n,0}f(R_-) = 0,\ f_0 = 0; \\ &\quad (-f'' + [(n-1)(n-3)/4]r^{-2}f) \in L^2((0,R);dr)\big\} \text{ for } n=2,3, \end{aligned} \tag{11.55}$$

$$\begin{aligned} &h^{(0)}_{n,\ell,\alpha_{n,\ell}} = -\frac{d^2}{dr^2} + \frac{4\kappa_{n,\ell} + (n-1)(n-3)}{4r^2}, \quad 0<r<R, \\ &\operatorname{dom}\big(h^{(0)}_{n,\ell,\alpha_{n,\ell}}\big) = \big\{f \in L^2((0,R);dr) \,\big|\, f,f' \in AC([\varepsilon,R]) \text{ for all } \varepsilon>0; \\ &\quad f'(R_-) + \alpha_{n,\ell}f(R_-) = 0; \\ &\quad (-f'' + [\kappa_{n,\ell} + ((n-1)(n-3)/4)]r^{-2}f) \in L^2((0,R);dr)\big\} \\ &\quad \text{for } \ell\in\mathbb{N},\ n\geq 2 \text{ and } \ell=0,\ n\geq 4. \end{aligned} \tag{11.56}$$

Here, in obvious notation, the boundary condition for $\alpha_{n,\ell}=\infty$ simply represents the Dirichlet boundary condition $f(R_-)=0$. In particular, the Friedrichs or

Dirichlet extension $h^{(0)}_{n,\ell,D}$ of $h^{(0)}_{n,\ell,\min}$ is given by $h^{(0)}_{n,\ell,\infty}$, that is, by

$$h^{(0)}_{n,0,D} = -\frac{d^2}{dr^2} + \frac{(n-1)(n-3)}{4r^2}, \quad 0 < r < R, \tag{11.57}$$
$$\operatorname{dom}\big(h^{(0)}_{n,0,D}\big) = \big\{f \in L^2((0,R);dr) \,\big|\, f, f' \in AC([\varepsilon,R]) \text{ for all } \varepsilon > 0;\ f(R_-) = 0,$$
$$f_0 = 0;\ (-f'' + [(n-1)(n-3)/4]r^{-2}f) \in L^2((0,R);dr)\big\} \text{ for } n = 2,3,$$

$$h^{(0)}_{n,\ell,D} = -\frac{d^2}{dr^2} + \frac{4\kappa_{n,\ell} + (n-1)(n-3)}{4r^2}, \quad 0 < r < R, \tag{11.58}$$
$$\operatorname{dom}\big(h^{(0)}_{n,\ell,D}\big) = \big\{f \in L^2((0,R);dr) \,\big|\, f, f' \in AC([\varepsilon,R]) \text{ for all } \varepsilon > 0;\ f(R_-) = 0;$$
$$(-f'' + [\kappa_{n,\ell} + ((n-1)(n-3)/4)]r^{-2}f) \in L^2((0,R);dr)\big\}$$
$$\text{for } \ell \in \mathbb{N},\ n \geq 2 \text{ and } \ell = 0,\ n \geq 4.$$

To find the boundary condition for the Krein–von Neumann extension $h^{(0)}_{n,\ell,K}$ of $h^{(0)}_{n,\ell,\min}$, that is, to find the corresponding boundary condition parameter $\alpha_{n,\ell,K}$ in (11.55), (11.56), we recall (2.10), that is,

$$\operatorname{dom}\big(h^{(0)}_{n,\ell,K}\big) = \operatorname{dom}\big(h^{(0)}_{n,\ell,\min}\big) \dotplus \ker\big(\big(h^{(0)}_{n,\ell,\min}\big)^*\big). \tag{11.59}$$

By inspection, the general solution of

$$\bigg(-\frac{d^2}{dr^2} + \frac{4\kappa_{n,\ell} + (n-1)(n-3)}{4r^2}\bigg)\psi(r) = 0, \quad r \in (0,R), \tag{11.60}$$

is given by

$$\psi(r) = Ar^{\ell+[(n-1)/2]} + Br^{-\ell-[(n-3)/2]}, \quad A, B \in \mathbb{C},\ r \in (0,R). \tag{11.61}$$

However, for $\ell \geq 1$, $n \geq 2$ and for $\ell = 0$, $n \geq 4$, the requirement $\psi \in L^2((0,R);dr)$ requires $B = 0$ in (11.61). Similarly, also the requirement $\psi_0 = 0$ (cf. (11.52)) for $\ell = 0$, $n = 2,3$, enforces $B = 0$ in (11.61).

Hence, any $u \in \operatorname{dom}\big(h^{(0)}_{n,\ell,K}\big)$ is of the type

$$u = f + \eta, \quad f \in \operatorname{dom}\big(h^{(0)}_{n,\ell,\min}\big), \quad \eta(r) = u(R_-)r^{\ell+[(n-1)/2]},\ r \in [0,R), \tag{11.62}$$

in particular, $f(R_-) = f'(R_-) = 0$. Denoting by $\alpha_{n,\ell,K}$ the boundary condition parameter for $h^{(0)}_{n,\ell,K}$ one thus computes

$$-\alpha_{n,\ell,K} = \frac{u'(R_-)}{u(R_-)} = \frac{\eta'(R_-)}{\eta(R_-)} = [\ell + ((n-1)/2)]/R. \tag{11.63}$$

Thus, the Krein–von Neumann extension $h^{(0)}_{n,\ell,K}$ of $h^{(0)}_{n,\ell,\min}$ is given by

$$\begin{aligned} h^{(0)}_{n,0,K} &= -\frac{d^2}{dr^2} + \frac{(n-1)(n-3)}{4r^2}, \quad 0<r<R, \\ \operatorname{dom}\big(h^{(0)}_{n,0,K}\big) &= \big\{f \in L^2((0,R);dr) \,\big|\, f,f' \in AC([\varepsilon,R]) \text{ for all } \varepsilon>0; \\ &\qquad f'(R_-) - [(n-1)/2]R^{-1}f(R_-) = 0,\ f_0 = 0; \\ &\qquad (-f'' + [(n-1)(n-3)/4]r^{-2}f) \in L^2((0,R);dr)\big\} \text{ for } n=2,3, \end{aligned} \tag{11.64}$$

$$\begin{aligned} h^{(0)}_{n,\ell,K} &= -\frac{d^2}{dr^2} + \frac{4\kappa_{n,\ell} + (n-1)(n-3)}{4r^2}, \quad 0<r<R, \\ \operatorname{dom}\big(h^{(0)}_{n,\ell,K}\big) &= \big\{f \in L^2((0,R);dr) \,\big|\, f,f' \in AC([\varepsilon,R]) \text{ for all } \varepsilon>0; \\ &\qquad f'(R_-) - [\ell + ((n-1)/2)]R^{-1}f(R_-) = 0; \\ &\qquad (-f'' + [\kappa_{n,\ell} + ((n-1)(n-3)/4)]r^{-2}f) \in L^2((0,R);dr)\big\} \\ &\qquad \text{for } \ell\in\mathbb{N},\ n\geq 2 \text{ and } \ell=0,\ n\geq 4. \end{aligned} \tag{11.65}$$

Next we briefly turn to the eigenvalues of $h^{(0)}_{n,\ell,D}$ and $h^{(0)}_{n,\ell,K}$. In analogy to (11.60), the solution ψ of

$$\bigg(-\frac{d^2}{dr^2} + \frac{4\kappa_{n,\ell} + (n-1)(n-3)}{4r^2} - z\bigg)\psi(r,z) = 0, \quad r\in(0,R), \tag{11.66}$$

satisfying the condition $\psi(\cdot,z) \in L^2((0,R);dr)$ for $\ell=0$, $n\geq 4$ and $\psi_0(z)=0$ (cf. (11.52)) for $\ell=0$, $n=2,3$, yields

$$\psi(r,z) = Ar^{1/2}J_{l+[(n-2)/2]}(z^{1/2}r), \quad A\in\mathbb{C},\ r\in(0,R), \tag{11.67}$$

Here $J_\nu(\cdot)$ denotes the Bessel function of the first kind and order ν (cf. [1, Sect. 9.1]). Thus, by the boundary condition $f(R_-)=0$ in (11.57), (11.58), the eigenvalues of the Dirichlet extension $h^{(0)}_{n,\ell,D}$ are determined by the equation $\psi(R_-,z)=0$, and hence by

$$J_{l+[(n-2)/2]}(z^{1/2}R) = 0. \tag{11.68}$$

Following [1, Sect. 9.5], we denote the zeros of $J_\nu(\cdot)$ by $j_{\nu,k}$, $k\in\mathbb{N}$, and hence obtain for the spectrum of $h^{(0)}_{n,\ell,F}$,

$$\sigma\big(h^{(0)}_{n,\ell,D}\big) = \big\{\lambda^{(0)}_{n,\ell,D,k}\big\}_{k\in\mathbb{N}} = \big\{j^2_{\ell+[(n-2)/2],k}R^{-2}\big\}_{k\in\mathbb{N}}, \quad \ell\in\mathbb{N}_0,\ n\geq 2. \tag{11.69}$$

Each eigenvalue of $h^{(0)}_{n,\ell,D}$ is simple.

Similarly, by the boundary condition $f'(R_-) - [\ell + ((n-1)/2)]R^{-1}f(R_-) = 0$ in (11.64), (11.65), the eigenvalues of the Krein–von Neumann extension $h^{(0)}_{n,\ell,K}$ are determined by the equation

$$\psi'(R,z) - [\ell + ((n-1)/2)]\psi(R,z) = -Az^{1/2}R^{1/2}J_{\ell+(n/2)}(z^{1/2}R) = 0 \tag{11.70}$$

(cf. [1, Eq. (9.1.27)]), and hence by

$$z^{1/2}J_{\ell+(n/2)}(z^{1/2}R) = 0. \tag{11.71}$$

Thus, one obtains for the spectrum of $h_{n,\ell,K}^{(0)}$,

$$\sigma\big(h_{n,\ell,K}^{(0)}\big) = \{0\} \cup \big\{\lambda_{n,\ell,K,k}^{(0)}\big\}_{k\in\mathbb{N}} = \{0\} \cup \big\{j_{\ell+(n/2),k}^2 R^{-2}\big\}_{k\in\mathbb{N}}, \quad \ell \in \mathbb{N}_0,\ n \geq 2. \tag{11.72}$$

Again, each eigenvalue of $h_{n,\ell,K}^{(0)}$ is simple, and $\eta(r) = Cr^{\ell+[(n-1)/2]}$, $C \in \mathbb{C}$, represents the (unnormalized) eigenfunction of $h_{n,\ell,K}^{(0)}$ corresponding to the eigenvalue 0.

Combining Propositions 2.2–2.4, one then obtains

$$-\Delta_{\max,B_n(0;R)} = (-\Delta_{\min,B_n(0;R)})^* = \bigoplus_{\ell\in\mathbb{N}_0} \big(H_{n,\ell,\min}^{(0)}\big)^* \otimes I_{\mathcal{K}_{n,\ell}}, \tag{11.73}$$

$$-\Delta_{D,B_n(0;R)} = \bigoplus_{\ell\in\mathbb{N}_0} H_{n,\ell,D}^{(0)} \otimes I_{\mathcal{K}_{n,\ell}}, \tag{11.74}$$

$$-\Delta_{K,B_n(0;R)} = \bigoplus_{\ell\in\mathbb{N}_0} H_{n,\ell,K}^{(0)} \otimes I_{\mathcal{K}_{n,\ell}}, \tag{11.75}$$

where (cf. (11.42))

$$H_{n,\ell,\max}^{(0)} = \big(H_{n,\ell,\min}^{(0)}\big)^* = U_n^{-1}\big(h_{n,\ell,\min}^{(0)}\big)^* U_n, \quad \ell \in \mathbb{N}_0, \tag{11.76}$$

$$H_{n,\ell,D}^{(0)} = U_n^{-1} h_{n,\ell,D}^{(0)} U_n, \quad \ell \in \mathbb{N}_0, \tag{11.77}$$

$$H_{n,\ell,K}^{(0)} = U_n^{-1} h_{n,\ell,K}^{(0)} U_n, \quad \ell \in \mathbb{N}_0. \tag{11.78}$$

Consequently,

$$\begin{aligned}\sigma(-\Delta_{D,B_n(0;R)}) &= \big\{\lambda_{n,\ell,D,k}^{(0)}\big\}_{\ell\in\mathbb{N}_0,k\in\mathbb{N}} \\ &= \big\{j_{\ell+[(n-2)/2],k}^2 R^{-2}\big\}_{\ell\in\mathbb{N}_0,k\in\mathbb{N}},\end{aligned} \tag{11.79}$$

$$\sigma_{\mathrm{ess}}(-\Delta_{D,B_n(0;R)}) = \emptyset, \tag{11.80}$$

$$\begin{aligned}\sigma(-\Delta_{K,B_n(0;R)}) &= \{0\} \cup \big\{\lambda_{n,\ell,K,k}^{(0)}\big\}_{\ell\in\mathbb{N}_0,k\in\mathbb{N}} \\ &= \{0\} \cup \big\{j_{\ell+(n/2),k}^2 R^{-2}\big\}_{\ell\in\mathbb{N}_0,k\in\mathbb{N}},\end{aligned} \tag{11.81}$$

$$\dim(\ker(-\Delta_{K,B_n(0;R)})) = \infty, \quad \sigma_{\mathrm{ess}}(-\Delta_{K,B_n(0;R)}) = \{0\}. \tag{11.82}$$

By (11.41), each eigenvalue $\lambda_{n,\ell,D,k}^{(0)}$, $k \in \mathbb{N}$, of $-\Delta_{D,B_n(0;R)}$ has multiplicity $d_{n,\ell}$ and similarly, again by (11.41), each eigenvalue $\lambda_{n,\ell,K,k}^{(0)}$, $k \in \mathbb{N}$, of $-\Delta_{K,B_n(0;R)}$ has multiplicity $d_{n,\ell}$.

Finally, we briefly turn to the Weyl asymptotics for the eigenvalue counting function (8.54) associated with the Krein Laplacian $-\Delta_{K,B_n(0;R)}$ for the ball $B_n(0;R)$, $R > 0$, in $\mathbb{R}^n$, $n \geq 2$. We will discuss a direct approach to the Weyl asymptotics that is independent of the general treatment presented in Section 9. Due to the smooth nature of the ball, we will obtain an improvement in the remainder term of the Weyl asymptotics of the Krein Laplacian.

First we recall the well-known fact that in the case of the Dirichlet Laplacian associated with the ball $B_n(0;R)$,

$$N^{(0)}_{D,B_n(0;R)}(\lambda) = (2\pi)^{-n} v_n^2 R^n \lambda^{n/2} - (2\pi)^{-(n-1)} v_{n-1}(n/4) v_n R^{n-1} \lambda^{(n-1)/2} + O\big(\lambda^{(n-2)/2}\big) \text{ as } \lambda \to \infty, \tag{11.83}$$

with $v_n = \pi^{n/2}/\Gamma((n/2)+1)$ the volume of the unit ball in $\mathbb{R}^n$ (and nv_n representing the surface area of the unit ball in $\mathbb{R}^n$).

Proposition 11.1. *The strictly positive eigenvalues of the Krein Laplacian associated with the ball of radius $R>0$, $B_n(0;R) \subset \mathbb{R}^n$, $R>0$, $n \geq 2$, satisfy the following Weyl-type eigenvalue asymptotics,*

$$N^{(0)}_{K,B_n(0;R)}(\lambda) = (2\pi)^{-n} v_n^2 R^n \lambda^{n/2} - (2\pi)^{-(n-1)} v_{n-1}[(n/4)v_n + v_{n-1}] R^{n-1} \lambda^{(n-1)/2} + O\big(\lambda^{(n-2)/2}\big) \text{ as } \lambda \to \infty. \tag{11.84}$$

Proof. From the outset one observes that

$$\lambda^{(0)}_{n,\ell,D,k} \leqslant \lambda^{(0)}_{n,\ell,K,k} \leqslant \lambda^{(0)}_{n,\ell,D,k+1}, \quad \ell \in \mathbb{N}_0,\ k \in \mathbb{N}, \tag{11.85}$$

implying

$$N^{(0)}_{K,B_n(0;R)}(\lambda) \leqslant N^{(0)}_{D,B_n(0;R)}(\lambda), \quad \lambda \in \mathbb{R}. \tag{11.86}$$

Next, introducing

$$\mathcal{N}_\nu(\lambda) := \begin{cases} \text{the largest } k \in \mathbb{N} \text{ such that } j_{\nu,k}^2 R^{-2} \leq \lambda, \\ 0, \text{ if no such } k \geq 1 \text{ exists,} \end{cases} \quad \lambda \in \mathbb{R}, \tag{11.87}$$

we note the well-known monotonicity of $j_{\nu,k}$ with respect to ν (cf. [184, Sect. 15.6, p. 508]), implying that for each $\lambda \in \mathbb{R}$ (and fixed $R>0$),

$$\mathcal{N}_{\nu'}(\lambda) \leq \mathcal{N}_\nu(\lambda) \text{ for } \nu' \geq \nu \geq 0. \tag{11.88}$$

Then one infers

$$N^{(0)}_{D,B_n(0;R)}(\lambda) = \sum_{\ell \in \mathbb{N}_0} d_{n,\ell}\, \mathcal{N}_{(n/2)-1+\ell}(\lambda), \quad N^{(0)}_{K,B_n(0;R)}(\lambda) = \sum_{\ell \in \mathbb{N}_0} d_{n,\ell}\, \mathcal{N}_{(n/2)+\ell}(\lambda). \tag{11.89}$$

Hence, using the fact that

$$d_{n,\ell} = d_{n-1,\ell} + d_{n,\ell-1} \tag{11.90}$$

(cf. (11.41)), setting $d_{n,-1} = 0$, $n \geq 2$, one computes

$$\begin{aligned} N^{(0)}_{D,B_n(0;R)}(\lambda) &= \sum_{\ell \in \mathbb{N}} d_{n,\ell-1}\, \mathcal{N}_{(n/2)-1+\ell}(\lambda) + \sum_{\ell \in \mathbb{N}_0} d_{n-1,\ell}\, \mathcal{N}_{(n/2)-1+\ell}(\lambda) \\ &\leq \sum_{\ell \in \mathbb{N}_0} d_{n,\ell}\, \mathcal{N}_{(n/2)+\ell}(\lambda) + \sum_{\ell \in \mathbb{N}_0} d_{n-1,\ell}\, \mathcal{N}_{((n-1)/2)-1+\ell}(\lambda) \\ &= N^{(0)}_{K,B_n(0;R)}(\lambda) + N^{(0)}_{D,B_{n-1}(0;R)}(\lambda), \end{aligned} \tag{11.91}$$

that is,

$$N^{(0)}_{D,B_n(0;R)}(\lambda) \leq N^{(0)}_{K,B_n(0;R)}(\lambda) + N^{(0)}_{D,B_{n-1}(0;R)}(\lambda). \tag{11.92}$$

Similarly,

$$\begin{aligned} N^{(0)}_{D,B_n(0;R)}(\lambda) &= \sum_{\ell\in\mathbb{N}} d_{n,\ell-1}\,\mathcal{N}_{(n/2)-1+\ell}(\lambda) + \sum_{\ell\in\mathbb{N}_0} d_{n-1,\ell}\,\mathcal{N}_{(n/2)-1+\ell}(\lambda) \\ &\geq \sum_{\ell\in\mathbb{N}_0} d_{n,\ell}\,\mathcal{N}_{(n/2)+\ell}(\lambda) + \sum_{\ell\in\mathbb{N}_0} d_{n-1,\ell}\,\mathcal{N}_{((n-1)/2)+\ell}(\lambda) \\ &= N^{(0)}_{K,B_n(0;R)}(\lambda) + N^{(0)}_{K,B_{n-1}(0;R)}(\lambda), \end{aligned} \tag{11.93}$$

that is,

$$N^{(0)}_{D,B_n(0;R)}(\lambda) \geq N^{(0)}_{K,B_n(0;R)}(\lambda) + N^{(0)}_{K,B_{n-1}(0;R)}(\lambda), \tag{11.94}$$

and hence,

$$N^{(0)}_{K,B_{n-1}(0;R)}(\lambda) \leq \big[N^{(0)}_{D,B_n(0;R)}(\lambda) - N^{(0)}_{K,B_n(0;R)}(\lambda)\big] \leq N^{(0)}_{D,B_{n-1}(0;R)}(\lambda). \tag{11.95}$$

Thus, using

$$\begin{aligned} 0 \leq \big[N^{(0)}_{D,B_n(0;R)}(\lambda) - N^{(0)}_{K,B_n(0;R)}(\lambda)\big] &\leq N^{(0)}_{D,B_{n-1}(0;R)}(\lambda) \\ &= O\big(\lambda^{(n-1)/2}\big) \ \text{ as } \lambda \to \infty, \end{aligned} \tag{11.96}$$

one first concludes that $\big[N^{(0)}_{D,B_n(0;R)}(\lambda) - N^{(0)}_{K,B_n(0;R)}(\lambda)\big] = O\big(\lambda^{(n-1)/2}\big)$ as $\lambda \to \infty$, and hence using (11.83),

$$N^{(0)}_{K,B_n(0;R)}(\lambda) = (2\pi)^{-n} v_n^2 R^n \lambda^{n/2} + O\big(\lambda^{(n-1)/2}\big) \ \text{ as } \ \lambda \to \infty. \tag{11.97}$$

This type of reasoning actually yields a bit more: Dividing (11.95) by $\lambda^{(n-1)/2}$, and using that both, $N^{(0)}_{D,B_{n-1}(0;R)}(\lambda)$ and $N^{(0)}_{K,B_{n-1}(0;R)}(\lambda)$ have the same leading asymptotics $(2\pi)^{-(n-1)} v_{n-1}^2 R^{n-1} \lambda^{(n-1)/2}$ as $\lambda \to \infty$, one infers, using (11.83) again,

$$\begin{aligned} N^{(0)}_{K,B_n(0;R)}(\lambda) &= N^{(0)}_{D,B_n(0;R)}(\lambda) - \big[N^{(0)}_{D,B_n(0;R)}(\lambda) - N^{(0)}_{K,B_n(0;R)}(\lambda)\big] \\ &= N^{(0)}_{D,B_n(0;R)}(\lambda) - (2\pi)^{-(n-1)} v_{n-1}^2 R^{n-1} \lambda^{(n-1)/2} + o\big(\lambda^{(n-1)/2}\big) \\ &= (2\pi)^{-n} v_n^2 R^n \lambda^{n/2} - (2\pi)^{-(n-1)} v_{n-1}[(n/4)v_n + v_{n-1}] R^{n-1} \lambda^{(n-1)/2} \\ &\quad + o\big(\lambda^{(n-1)/2}\big) \ \text{ as } \lambda \to \infty. \end{aligned} \tag{11.98}$$

Finally, it is possible to improve the remainder term in (11.98) from $o\big(\lambda^{(n-1)/2}\big)$ to $O\big(\lambda^{(n-2)/2}\big)$ as follows: Replacing n by $n-1$ in (11.92) yields

$$N^{(0)}_{D,B_{n-1}(0;R)}(\lambda) \leq N^{(0)}_{K,B_{n-1}(0;R)}(\lambda) + N^{(0)}_{D,B_{n-2}(0;R)}(\lambda). \tag{11.99}$$

Insertion of (11.99) into (11.94) permits one to eliminate $N^{(0)}_{K,B_{n-1}(0;R)}$ as follows:

$$N^{(0)}_{D,B_n(0;R)}(\lambda) \geq N^{(0)}_{K,B_n(0;R)}(\lambda) + N^{(0)}_{D,B_{n-1}(0;R)}(\lambda) - N^{(0)}_{D,B_{n-2}(0;R)}(\lambda), \tag{11.100}$$

which implies

$$\begin{aligned}&\big[N^{(0)}_{D,B_n(0;R)}(\lambda) - N^{(0)}_{D,B_{n-1}(0;R)}(\lambda)\big] \leq N^{(0)}_{K,B_n(0;R)}(\lambda)\\&\quad\leq \big[N^{(0)}_{D,B_n(0;R)}(\lambda) - N^{(0)}_{D,B_{n-1}(0;R)}(\lambda)\big] + N^{(0)}_{D,B_{n-2}(0;R)}(\lambda),\end{aligned} \tag{11.101}$$

and hence,

$$0 \leq N^{(0)}_{K,B_n(0;R)}(\lambda) - \big[N^{(0)}_{D,B_n(0;R)}(\lambda) - N^{(0)}_{D,B_{n-1}(0;R)}(\lambda)\big] \leq N^{(0)}_{D,B_{n-2}(0;R)}(\lambda). \tag{11.102}$$

Thus, $N^{(0)}_{K,B_n(0;R)}(\lambda) - \big[N^{(0)}_{D,B_n(0;R)}(\lambda) - N^{(0)}_{D,B_{n-1}(0;R)}(\lambda)\big] = O\big(\lambda^{(n-2)/2}\big)$ as $\lambda \to \infty$, proving (11.84). □

Due to the smoothness of the domain $B_n(0;R)$, the remainder terms in (11.84) represent a marked improvement over the general result (9.13) for domains Ω satisfying Hypothesis 6.2. A comparison of the second term in the asymptotic relations (11.83) and (11.84) exhibits the difference between Dirichlet and Krein–von Neumann eigenvalues.

11.4. The case $\Omega = \mathbb{R}^n\backslash\{0\}$, $n = 2, 3$, $V = 0$

In this subsection we consider the following minimal operator $-\Delta_{\min,\mathbb{R}^n\backslash\{0\}}$ in $L^2(\mathbb{R}^n; d^n x)$, $n = 2, 3$,

$$-\Delta_{\min,\mathbb{R}^n\backslash\{0\}} = \overline{-\Delta\big|_{C_0^\infty(\mathbb{R}^n\backslash\{0\})}} \geq 0, \quad n = 2, 3. \tag{11.103}$$

Then

$$\begin{aligned}&H_{F,\mathbb{R}^2\backslash\{0\}} = H_{K,\mathbb{R}^2\backslash\{0\}} = -\Delta,\\&\operatorname{dom}(H_{F,\mathbb{R}^2\backslash\{0\}}) = \operatorname{dom}(H_{K,\mathbb{R}^2\backslash\{0\}}) = H^2(\mathbb{R}^2) \ \text{ if } \ n = 2\end{aligned} \tag{11.104}$$

is the unique nonnegative self-adjoint extension of $-\Delta_{\min,\mathbb{R}^2\backslash\{0\}}$ in $L^2(\mathbb{R}^2; d^2x)$ and

$$\begin{aligned}&H_{F,\mathbb{R}^3\backslash\{0\}} = H_{D,\mathbb{R}^3\backslash\{0\}} = -\Delta,\\&\operatorname{dom}(H_{F,\mathbb{R}^3\backslash\{0\}}) = \operatorname{dom}(H_{D,\mathbb{R}^3\backslash\{0\}}) = H^2(\mathbb{R}^3) \ \text{ if } \ n = 3,\end{aligned} \tag{11.105}$$

$$H_{K,\mathbb{R}^3\backslash\{0\}} = H_{N,\mathbb{R}^3\backslash\{0\}} = U^{-1}h^{(0)}_{0,N,\mathbb{R}_+}U \oplus \bigoplus_{\ell\in\mathbb{N}} U^{-1}h^{(0)}_{\ell,\mathbb{R}_+}U \ \text{ if } \ n = 3, \tag{11.106}$$

where $H_{D,\mathbb{R}^3\backslash\{0\}}$ and $H_{N,\mathbb{R}^3\backslash\{0\}}$ denote the Dirichlet and Neumann[1] extension of $-\Delta_{\min,\mathbb{R}^n\backslash\{0\}}$ in $L^2(\mathbb{R}^3; d^3x)$, respectively. Here we used the angular momentum

[1] The Neumann extension $H_{N,\mathbb{R}^3\backslash\{0\}}$ of $-\Delta_{\min,\mathbb{R}^n\backslash\{0\}}$, associated with a Neumann boundary condition, in honor of Carl Gottfried Neumann, should of course not be confused with the Krein–von Neumann extension $H_{K,\mathbb{R}^3\backslash\{0\}}$ of $-\Delta_{\min,\mathbb{R}^n\backslash\{0\}}$.

decomposition (cf. also (11.39), (11.40)),

$$\begin{aligned} L^2(\mathbb{R}^n; d^n x) &= L^2((0,\infty); r^{n-1}dr) \otimes L^2(S^{n-1}; d\omega_{n-1}) \\ &= \bigoplus_{\ell\in\mathbb{N}_0} \mathcal{H}_{n,\ell,(0,\infty)}, \end{aligned} \tag{11.107}$$

$$\mathcal{H}_{n,\ell,(0,\infty)} = L^2((0,\infty); r^{n-1}dr) \otimes \mathcal{K}_{n,\ell}, \quad \ell \in \mathbb{N}_0,\ n = 2,3. \tag{11.108}$$

Moreover, we abbreviated $\mathbb{R}_+ = (0,\infty)$ and introduced

$$\begin{aligned} &h^{(0)}_{0,N,\mathbb{R}_+} = -\frac{d^2}{dr^2}, \quad r > 0, \\ &\operatorname{dom}\big(h^{(0)}_{0,N,\mathbb{R}_+}\big) = \big\{f \in L^2((0,\infty); dr) \,\big|\, f, f' \in AC([0,R]) \text{ for all } R > 0; \\ &\qquad\qquad f'(0_+) = 0;\ f'' \in L^2((0,\infty); dr)\big\}, \end{aligned} \tag{11.109}$$

$$\begin{aligned} &h^{(0)}_{\ell,\mathbb{R}_+} = -\frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{r^2}, \quad r > 0, \\ &\operatorname{dom}\big(h^{(0)}_{\ell,\mathbb{R}_+}\big) = \big\{f \in L^2((0,\infty); dr) \,\big|\, f, f' \in AC([0,R]) \text{ for all } R > 0; \\ &\qquad\qquad - f'' + \ell(\ell+1)r^{-2}f \in L^2((0,\infty); dr)\big\}, \quad \ell \in \mathbb{N}. \end{aligned} \tag{11.110}$$

The operators $h^{(0)}_{\ell,\mathbb{R}_+}|_{C_0^\infty((0,\infty))}$, $\ell \in \mathbb{N}$, are essentially self-adjoint in $L^2((0,\infty); dr)$ (but we note that $f \in \operatorname{dom}\big(h^{(0)}_{\ell,\mathbb{R}_+}\big)$ implies that $f(0_+) = 0$). In addition, U in (11.106) denotes the unitary operator,

$$U : \begin{cases} L^2((0,\infty); r^2dr) \to L^2((0,\infty); dr), \\ \qquad\qquad f(r) \mapsto (Uf)(r) = rf(r). \end{cases} \tag{11.111}$$

As discussed in detail in [83, Sects. 4, 5], equations (11.104)–(11.106) follow from Corollary 4.8 in [83] and the facts that

$$(u_+, M_{H_{F,\mathbb{R}^n\setminus\{0\}},\mathcal{N}_+}(z)u_+)_{L^2(\mathbb{R}^n;d^nx)} = \begin{cases} -(2/\pi)\ln(z) + 2i, & n = 2, \\ i(2z)^{1/2} + 1, & n = 3, \end{cases} \tag{11.112}$$

and

$$(u_+, M_{H_{K,\mathbb{R}^3\setminus\{0\}},\mathcal{N}_+}(z)u_+)_{L^2(\mathbb{R}^3;d^3x)} = i(2/z)^{1/2} - 1. \tag{11.113}$$

Here

$$\begin{aligned} &\mathcal{N}_+ = \operatorname{lin.span}\{u_+\}, \\ &u_+(x) = G_0(i,x,0)/\|G_0(i,\cdot,0)\|_{L^2(\mathbb{R}^n;d^nx)},\ x \in \mathbb{R}^n\backslash\{0\},\ n = 2,3, \end{aligned} \tag{11.114}$$

and

$$G_0(z,x,y) = \begin{cases} \frac{i}{4}H_0^{(1)}(z^{1/2}|x-y|), & x \neq y,\ n = 2, \\ e^{iz^{1/2}|x-y|}/(4\pi|x-y|), & x \neq y,\ n = 3 \end{cases} \tag{11.115}$$

denotes the Green's function of $-\Delta$ defined on $H^2(\mathbb{R}^n)$, $n = 2,3$ (i.e., the integral kernel of the resolvent $(-\Delta - z)^{-1}$), and $H_0^{(1)}(\cdot)$ abbreviates the Hankel function of the first kind and order zero (cf., [1, Sect. 9.1]). Here the Donoghue-type Weyl–Titchmarsh operators (cf. [70] in the case where $\dim(\mathcal{N}_+) = 1$ and [83], [85], and [91] in the general abstract case where $\dim(\mathcal{N}_+) \in \mathbb{N} \cup \{\infty\}$) $M_{H_{F,\mathbb{R}^n\setminus\{0\}},\mathcal{N}_+}$ and $M_{H_{K,\mathbb{R}^n\setminus\{0\}},\mathcal{N}_+}$ are defined according to equation (4.8) in [83]: More precisely, given a self-adjoint extension $\widetilde{S}$ of the densely defined closed symmetric operator S in a complex separable Hilbert space $\mathcal{H}$, and a closed linear subspace $\mathcal{N}$ of $\mathcal{N}_+ = \ker(S^* - iI_{\mathcal{H}})$, $\mathcal{N} \subseteq \mathcal{N}_+$, the Donoghue-type Weyl–Titchmarsh operator $M_{\widetilde{S},\mathcal{N}}(z) \in \mathcal{B}(\mathcal{N})$ associated with the pair $(\widetilde{S}, \mathcal{N})$ is defined by

$$\begin{aligned} M_{\widetilde{S},\mathcal{N}}(z) &= P_{\mathcal{N}}(z\widetilde{S} + I_{\mathcal{H}})(\widetilde{S} - zI_{\mathcal{H}})^{-1}P_{\mathcal{N}}\big|_{\mathcal{N}} \\ &= zI_{\mathcal{N}} + (1+z^2)P_{\mathcal{N}}(\widetilde{S} - zI_{\mathcal{H}})^{-1}P_{\mathcal{N}}\big|_{\mathcal{N}}, \quad z \in \mathbb{C}\backslash\mathbb{R}, \end{aligned} \tag{11.116}$$

with $I_{\mathcal{N}}$ the identity operator in $\mathcal{N}$ and $P_{\mathcal{N}}$ the orthogonal projection in $\mathcal{H}$ onto $\mathcal{N}$.

Equation (11.112) then immediately follows from repeated use of the identity (the first resolvent equation),

$$\begin{aligned} \int_{\mathbb{R}^n} d^n x' G_0(z_1, x, x') G_0(z_2, x', 0) = (z_1 - z_2)^{-1}[G_0(z_1, x, 0) - G_0(z_2, x, 0)], \\ x \neq 0,\ z_1 \neq z_2,\ n = 2, 3, \end{aligned} \tag{11.117}$$

and its limiting case as $x \to 0$.

Finally, (11.113) follows from the following arguments: First one notices that

$$\big[-(d^2/dr^2) + \alpha\, r^{-2}\big]\big|_{C_0^\infty((0,\infty))} \tag{11.118}$$

is essentially self-adjoint in $L^2(\mathbb{R}_+; dr)$ if and only if $\alpha \geq 3/4$. Hence it suffices to consider the restriction of $H_{\min,\mathbb{R}^3\setminus\{0\}}$ to the centrally symmetric subspace $\mathcal{H}_{3,0,(0,\infty)}$ of $L^2(\mathbb{R}^3; d^3x)$ corresponding to angular momentum $\ell = 0$ in (11.107), (11.108). But then it is a well-known fact (cf. [83, Sects. 4, 5]) that the Donoghue-type Dirichlet m-function $(u_+, M_{H_{D,\mathbb{R}^3\setminus\{0\}},\mathcal{N}_+}(z)u_+)_{L^2(\mathbb{R}^3;d^3x)}$, satisfies

$$\begin{aligned} (u_+, M_{H_{D,\mathbb{R}^3\setminus\{0\}},\mathcal{N}_+}(z)u_+)_{L^2(\mathbb{R}^3;d^3x)} &= (u_{0,+}, M_{h^{(0)}_{0,D,\mathbb{R}_+},\mathcal{N}_{0,+}}(z)u_{0,+})_{L^2(\mathbb{R}_+;dr)}, \\ &= i(2z)^{1/2} + 1, \end{aligned} \tag{11.119}$$

where

$$\mathcal{N}_{0,+} = \operatorname{lin.span}\{u_{0,+}\}, \quad u_{0,+}(r) = e^{iz^{1/2}r}/[2\operatorname{Im}(z^{1/2}]^{1/2},\ r > 0, \tag{11.120}$$

and $M_{h^{(0)}_{0,D,\mathbb{R}_+},\mathcal{N}_{0,+}}(z)$ denotes the Donoghue-type Dirichlet m-function corresponding to the operator

$$\begin{aligned} & h^{(0)}_{0,D,\mathbb{R}_+} = -\frac{d^2}{dr^2}, \quad r > 0, \\ & \operatorname{dom}\big(h^{(0)}_{0,D,\mathbb{R}_+}\big) = \big\{f \in L^2((0,\infty); dr) \,\big|\, f, f' \in AC([0,R]) \text{ for all } R > 0; \\ & \qquad\qquad f(0_+) = 0;\ f'' \in L^2((0,\infty); dr)\big\}, \end{aligned} \tag{11.121}$$

Next, turning to the Donoghue-type Neumann m-function given by

$$(u_+, M_{H_{N,\mathbb{R}^3\setminus\{0\}},\mathcal{N}_+}(z)u_+)_{L^2(\mathbb{R}^3;d^3x)}$$

one obtains analogously to (11.119) that

$$(u_+, M_{H_{N,\mathbb{R}^3\backslash\{0\}},\mathcal{N}_+}(z)u_+)_{L^2(\mathbb{R}^3;d^3x)} = (u_{0,+}, M_{h^{(0)}_{0,N,\mathbb{R}_+},\mathcal{N}_{0,+}}(z)u_{0,+})_{L^2(\mathbb{R}_+;dr)}, \tag{11.122}$$

where $M_{h^{(0)}_{0,N,\mathbb{R}_+},\mathcal{N}_{0,+}}(z)$ denotes the Donoghue-type Neumann m-function corresponding to the operator $h^{(0)}_{0,N,\mathbb{R}_+}$ in (11.109). The well-known linear fractional transformation relating the operators $M_{h^{(0)}_{0,D,\mathbb{R}_+},\mathcal{N}_{0,+}}(z)$ and $M_{h^{(0)}_{0,N,\mathbb{R}_+},\mathcal{N}_{0,+}}(z)$ (cf. [83, Lemmas 5.3, 5.4, Theorem 5.5, and Corollary 5.6]) then yields

$$(u_{0,+}, M_{h^{(0)}_{0,N,\mathbb{R}_+},\mathcal{N}_{0,+}}(z)u_{0,+})_{L^2(\mathbb{R}_+;dr)} = i(2/z)^{1/2} - 1, \tag{11.123}$$

verifying (11.113).

The fact that the operator $T = -\Delta$, $\operatorname{dom}(T) = H^2(\mathbb{R}^2)$ is the unique nonnegative self-adjoint extension of $-\Delta_{\min,\mathbb{R}^2\backslash\{0\}}$ in $L^2(\mathbb{R}^2; d^2x)$, has been shown in [12] (see also [13, Ch. I.5]).

11.5. The case $\Omega = \mathbb{R}^n\backslash\{0\}$, $V = -[(n-2)^2/4]|x|^{-2}$, $n \geq 2$

In our final subsection we briefly consider the following minimal operator $H_{\min,\mathbb{R}^n\backslash\{0\}}$ in $L^2(\mathbb{R}^n; d^nx)$, $n \geq 2$,

$$H_{\min,\mathbb{R}^n\backslash\{0\}} = \overline{(-\Delta - ((n-2)^2/4)|x|^{-2})\big|_{C_0^\infty(\mathbb{R}^n\backslash\{0\})}} \geq 0, \quad n \geq 2. \tag{11.124}$$

Then, using again the angular momentum decomposition (cf. also (11.39), (11.40)),

$$L^2(\mathbb{R}^n; d^nx) = L^2((0,\infty); r^{n-1}dr) \otimes L^2(S^{n-1}; d\omega_{n-1}) = \bigoplus_{\ell\in\mathbb{N}_0} \mathcal{H}_{n,\ell,(0,\infty)}, \tag{11.125}$$

$$\mathcal{H}_{n,\ell,(0,\infty)} = L^2((0,\infty); r^{n-1}dr) \otimes \mathcal{K}_{n,\ell}, \quad \ell \in \mathbb{N}_0,\ n \geq 2, \tag{11.126}$$

one finally obtains that

$$H_{F,\mathbb{R}^n\backslash\{0\}} = H_{K,\mathbb{R}^n\backslash\{0\}} = U^{-1}h_{0,\mathbb{R}_+}U \oplus \bigoplus_{\ell\in\mathbb{N}} U^{-1}h_{n,\ell,\mathbb{R}_+}U,\ n \geq 2, \tag{11.127}$$

is the unique nonnegative self-adjoint extension of $H_{\min,\mathbb{R}^n\backslash\{0\}}$ in $L^2(\mathbb{R}^n; d^nx)$, where

$$\begin{aligned} &h_{0,\mathbb{R}_+} = -\frac{d^2}{dr^2} - \frac{1}{4r^2}, \quad r > 0, \\ &\operatorname{dom}(h_{0,\mathbb{R}_+}) = \big\{f \in L^2((0,\infty); dr) \,\big|\, f, f' \in AC([\varepsilon, R]) \text{ for all } 0 < \varepsilon < R; \\ &\qquad\qquad f_0 = 0;\ (-f'' - (1/4)r^{-2}f) \in L^2((0,\infty); dr)\big\}, \end{aligned} \tag{11.128}$$

$$\begin{aligned} &h_{n,\ell,\mathbb{R}_+} = -\frac{d^2}{dr^2} + \frac{4\kappa_{n,\ell} - 1}{4r^2}, \quad r > 0, \\ &\operatorname{dom}(h_{n,\ell,\mathbb{R}_+}) = \big\{f \in L^2((0,\infty); dr) \,\big|\, f, f' \in AC([\varepsilon, R]) \text{ for all } 0 < \varepsilon < R; \\ &\qquad (-f'' + [\kappa_{n,\ell} - (1/4)]r^{-2}f) \in L^2((0,\infty); dr)\big\}, \quad \ell \in \mathbb{N},\ n \geq 2. \end{aligned} \tag{11.129}$$

Here f_0 in (11.128) is defined by (cf. also (11.51))

$$f_0 = \lim_{r \downarrow 0} [-r^{1/2} \ln(r)]^{-1} f(r). \tag{11.130}$$

As in the previous subsection, $h_{n,\ell,\mathbb{R}_+}|_{C_0^\infty((0,\infty))}$, $\ell \in \mathbb{N}$, $n \geq 2$, are essentially self-adjoint in $L^2((0,\infty); dr)$. In addition, $h_{0,\mathbb{R}_+}$ is the unique nonnegative self-adjoint extension of $h_{0,\mathbb{R}_+}|_{C_0^\infty((0,\infty))}$ in $L^2((0,\infty); dr)$. We omit further details.

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Eigenvalues of Non-selfadjoint Operators: A Comparison of Two Approaches

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Abstract. The central problem we consider is the distribution of eigenvalues of closed linear operators which are not selfadjoint, with a focus on those operators which are obtained as perturbations of selfadjoint linear operators. Two methods are explained and elaborated. One approach uses complex analysis to study a holomorphic function whose zeros can be identified with the eigenvalues of the linear operator. The second method is an operator theoretic approach involving the numerical range. General results obtained by the two methods are derived and compared. Applications to non-selfadjoint Jacobi and Schrödinger operators are considered. Some possible directions for future research are discussed.

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1. Introduction

The importance of eigenvalues and eigenvectors is clear to every student of mathematics, science or engineering. As a simple example, consider a linear dynamical system which is described by an equation of the form

$$u_t = Lu, \tag{1.1}$$

where $u(t)$ is an element in a linear space X and L a linear operator in X. If we can find an eigenpair $v \in X$, $\lambda \in \mathbb{C}$ with $Lv = \lambda v$, then we have solved (1.1) with the initial condition $u(0) = v$: $u(t) = e^{\lambda t} v$. If we can find a whole basis of eigenvectors, we have solved (1.1) for any initial condition $u(0) = u_0$ by decomposing u_0 with respect to this basis. So the knowledge of the eigenvalues of L (or more generally, the analysis of its spectrum) is essential for the understanding of the corresponding system.

The *spectral analysis* of linear operators has a quite long history, as everybody interested in the field is probably aware of. Still, we think that it can be worthwhile to begin this introduction with a short historical survey, which will also help to put the present article in its proper perspective. The origins of spectral analysis can be traced back at least as far as the work of D'Alembert and Euler (1740–50's) on vibrating strings, where eigenvalues correspond to frequencies of vibration, and eigenvectors correspond to modes of vibration. When the vibrating string's density and tension are not uniform, the eigenvalue problem involved becomes much more challenging, and an early landmark of spectral theory is Sturm and Liouville's (1836–1837) analysis of general one-dimensional problems on bounded intervals, showing the existence of an infinite sequence of eigenvalues. This naturally gave rise to questions about corresponding results for differential operators on higher-dimensional domains, with the typical problem being the eigenvalues of the Laplacian on a bounded domain with Dirichlet boundary conditions. The existence of the first eigenvalue for this problem was obtained by Schwartz (1885), and of the second eigenvalue by Picard (1893), and it was Poincaré (1894) who obtained existence of all eigenvalues and their basic properties. Inspired by Poincarés work, Fredholm (1903) undertook the study of the spectral theory of integral operators. Hilbert (1904–1910), generalizing the work of Fredholm, introduced the ideas of quadratic forms on infinite-dimensional linear spaces and of completely continuous forms (compact operators in current terminology). He also realized that spectral analysis cannot be performed in terms of eigenvalues alone, developing the notion of continuous spectrum, which was prefigured in Wirtinger's (1897) work on Hill's equation. Weyl's (1908) work on integral equations on unbounded intervals further stresses the importance of the continuous spectrum. The advent of quantum mechanics, formulated axiomatically by von Neumann (1927), who was the first to introduce the notion of an abstract Hilbert space, brought selfadjoint operators into the forefront of interest. Kato's [31] rigorous proof of the selfadjointness of physically relevant Schrödinger operators was a starting point for the mathematical study of particular operators. In the context of quantum mechanics, eigenvalues have special significance, as they correspond to discrete energy levels, and thus form the basis for the quantization phenomenon, which in the pre-Schrödinger quantum theory had to be postulated a priori. In recent years, non-selfadjoint operators are also becoming increasingly important in the study of quantum mechanical systems, as they arise naturally in, e.g., the optical model of nuclear scattering or the study of the behavior of unstable lasers (see [8] and references therein).

As this brief sketch[1] of some highlights of the (early) history of spectral theory shows, eigenvalues, eigenvectors, and the spectrum provide an endless source of fascination for both mathematicians and physicists. At the most general level one may ask, given a class $\mathcal{C}$ of linear operators (which in our case will always operate in a Hilbert space), what can be said about the spectrum of operators $L \in \mathcal{C}$? Of course, the more restricted is the class of operators considered the more we

[1]The interested reader can find much more information (and detailed references) in Mawhin's account [37] on the origins of spectral analysis.

can say, and the techniques available for studying different classes $\mathcal{C}$ can vary enormously. For example, an important part of the work of Hilbert is a theory of selfadjoint compact operators, which in particular characterizes their spectrum as an infinite sequence of real eigenvalues. Motivated by various applications, this class of operators can be restricted or broadened to yield other classes worth studying. For example, the study of eigenvalues of the Dirichlet problem in a bounded domain is a restriction of the class of compact selfadjoint eigenvalue problems, which yields a rich theory relating the eigenvalues to the geometrical properties of the domain in question. As far as broadening the class of operators goes, one can consider selfadjoint operators which are not compact, leading to a vast domain of study which is of great importance to a variety of areas of application, perhaps the most prominent being quantum mechanics. One can also consider compact operators which are not selfadjoint (and which might act in general Banach spaces), leading to a field of research in which natural sub-classes of the class of compact operators are defined and their sets of eigenvalues are studied (see, e.g., the classical works of Gohberg and Krein [21] or Pietsch [38]).

One may also lift both the assumption of selfadjointness *and* that of compactness. However, *some* restriction on the class of operators considered must be made in order to be able to say anything nontrivial about the spectrum. The classes of operators that we will be considering here are those that arise by perturbing bounded or unbounded (in most cases selfadjoint) operators with no isolated eigenvalues by operators which are (relatively) compact, for example operators of the form $A = A_0 + M$, where A_0 is a bounded operator with spectrum $\sigma(A_0) = [a, b]$ and M is a compact operator in a certain Schatten class. More precisely, we will be interested in the isolated eigenvalues of such operators A and in their rate of accumulation to the essential spectrum $[a, b]$. We will study this rate by analyzing eigenvalue moments of the form

$$\sum_{\lambda \in \sigma_d(A)} (\mathrm{dist}(\lambda, [a, b]))^p, \qquad p > 0, \tag{1.2}$$

where $\sigma_d(A)$ is the set of discrete eigenvalues, and by bounding these moments in terms of the Schatten norm of the perturbation M.

It is well known that the summation of two ‘simple’ operators can generate an operator whose spectrum is quite difficult to understand, even in case that both operators are selfadjoint. In our case, at least one of the operators will be non-selfadjoint, so the huge toolbox of the selfadjoint theory (containing, e.g., the spectral theorem, the decomposition of the spectrum into its various parts or the variational characterization of the eigenvalues) will not be available. This will make the problem even more demanding and also indicates that we cannot expect to obtain as much information on the spectrum as in the selfadjoint case. At this point we cannot resist quoting E.B. Davies, who in the preface of his book [8] on the spectral theory of non-selfadjoint operators described the differences between the selfadjoint and the non-selfadjoint theory: “Studying non-selfadjoint operators is like being a vet rather than a doctor: one has to acquire a much wider range of knowledge, and to accept that one cannot expect to have as high a rate of success when confronted with particular cases".

In our previous work, which we review in this paper, we have developed and explored two quite different approaches to obtain results on the distribution of eigenvalues of non-selfadjoint operators. One approach, which has also benefitted from (and relies heavily on) some related work of Borichev, Golinskii and Kupin [5], involves the construction of a holomorphic function whose zeros coincide with the eigenvalues of the operator of interest (the 'perturbation determinant') and the study of these zeros by employing results of complex analysis. The second is an operator-theoretic approach using the concept of numerical range. One of our main aims in this paper is to present these two methods side by side, and to examine the advantages of each of them in terms of the results they yield. We shall see that each of these methods has certain advantages over the other.

The plan of this paper is as follows. In Chapter 2 we recall fundamental concepts and results of functional analysis and operator theory that will be used. In Chapter 3 we discuss results on zeros of complex functions that will later be used to obtain results on eigenvalues. In particular, we begin this chapter with a short explanation why results from complex analysis can be used to obtain estimates on eigenvalue moments of the form (1.2) in the first place. Next, in Chapter 4, we develop the complex-analysis approach to obtaining results on eigenvalues of perturbed operators, obtaining results of varying degrees of generality for Schatten-class perturbations of selfadjoint bounded operators and for relatively-Schatten perturbations of non-negative operators. A second, independent, approach to obtaining eigenvalue estimates via operator-theoretic arguments is exposed in Chapter 5, and applied to the same classes of operators. In Chapter 6 we carry out a detailed comparison of the results obtained by the two approaches in the context of Schatten-perturbations of bounded selfadjoint operators. In Chapter 7 we turn to applications of the results obtained in Chapter 4 and 5 to some concrete classes of operators, which allows us to further compare the results obtained by the two approaches in these specific contexts. We obtain results on the eigenvalues of Jacobi operators and of Schrödinger operators with complex potentials. These case-studies also give us the opportunity to compare the results obtained by our methods to results which have been obtained by other researchers using different methods. These comparisons give rise to some conjectures and open questions which we believe could stimulate further research. Some further directions of ongoing work related to the work discussed in this paper, and issues that we believe are interesting to address, are discussed in Chapter 8. A list of symbols is provided on page 160.

2. Preliminaries

In this chapter we will introduce and review some basic concepts of operator and spectral theory, restricting ourselves to those aspects of the theory which are relevant in the later parts of this work. We will also use this chapter to set our notation and terminology. As general references let us mention the monographs of Davies [8], Gohberg, Goldberg and Kaashoek [19], Gohberg and Krein [21] and Kato [33].

2.1. The spectrum of linear operators

Let $\mathcal{H}$ denote a complex separable Hilbert space and let Z be a linear operator in $\mathcal{H}$. The domain, range and kernel of Z are denoted by $\mathrm{Dom}(Z)$, $\mathrm{Ran}(Z)$ and $\mathrm{Ker}(Z)$, respectively. We say that Z is an operator *on* $\mathcal{H}$ if $\mathrm{Dom}(Z) = \mathcal{H}$. The algebra of all bounded operators on $\mathcal{H}$ is denoted by $\mathcal{B}(\mathcal{H})$. Similarly, $\mathcal{C}(\mathcal{H})$ denotes the class of all closed operators in $\mathcal{H}$.

In the following we assume that Z is a closed operator in $\mathcal{H}$. The resolvent set of Z is defined as

$$\rho(Z) := \{\lambda \in \mathbb{C} : \lambda - Z \text{ is invertible in } \mathcal{B}(\mathcal{H})\}^2 \tag{2.1.1}$$

and for $\lambda \in \rho(Z)$ we define

$$R_Z(\lambda) := (\lambda - Z)^{-1}. \tag{2.1.2}$$

The complement of $\rho(Z)$ in $\mathbb{C}$, denoted by $\sigma(Z)$, is called the spectrum of Z. Note that $\rho(Z)$ is an open and $\sigma(Z)$ is a closed subset of $\mathbb{C}$. We say that $\lambda \in \sigma(Z)$ is an eigenvalue of Z if $\mathrm{Ker}(\lambda - Z)$ is nontrivial.

The extended resolvent set of Z is defined as

$$\hat{\rho}(Z) := \begin{cases} \rho(Z) \cup \{\infty\}, & \text{if } Z \in \mathcal{B}(\mathcal{H}) \\ \rho(Z), & \text{if } Z \notin \mathcal{B}(\mathcal{H}). \end{cases} \tag{2.1.3}$$

In particular, if $Z \in \mathcal{B}(\mathcal{H})$ we regard $\hat{\rho}(Z)$ as a subset of the extended complex plane $\hat{\mathbb{C}} = \mathbb{C} \cup \{\infty\}$. Setting $R_Z(\infty) := 0$ if $Z \in \mathcal{B}(\mathcal{H})$, the operator-valued function

$$R_Z : \lambda \mapsto R_Z(\lambda),$$

called the resolvent of Z, is analytic on $\hat{\rho}(Z)$. Moreover, for every $\lambda \in \hat{\rho}(Z)$ the resolvent satisfies the inequality $\|R_Z(\lambda)\| \geq \mathrm{dist}(\lambda, \sigma(Z))^{-1}$, where $\|.\|$ denotes the norm of $\mathcal{B}(\mathcal{H})$[3] and we agree that $1/\infty := 0$. Actually, if Z is a normal operator (that is, an operator commuting with its adjoint) then the spectral theorem implies that

$$\|R_Z(\lambda)\| = \mathrm{dist}(\lambda, \sigma(Z))^{-1}, \quad \lambda \in \hat{\rho}(Z). \tag{2.1.4}$$

If $\lambda \in \sigma(Z)$ is an isolated point of the spectrum, we define the Riesz projection of Z with respect to λ by

$$P_Z(\lambda) := \frac{1}{2\pi i} \int_\gamma R_Z(\mu) d\mu, \tag{2.1.5}$$

where the contour γ is a counterclockwise oriented circle centered at λ, with sufficiently small radius (excluding the rest of $\sigma(Z)$). We recall that a subspace $M \subset \mathcal{H}$

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[2]Note that here and elsewhere in the text, we use $\lambda - Z$ as a shorthand for $\lambda I - Z$ where I denotes the identity operator on $\mathcal{H}$.

[3]We will use the same symbol to denote the norm on $\mathcal{H}$.

is called Z-invariant if $Z(M \cap \mathrm{Dom}(Z)) \subset M$. In this case, $Z|_M$ denotes the restriction of Z to $M \cap \mathrm{Dom}(Z)$ and the range of $Z|_M$ is a subspace of M.

Proposition 2.1.1 (see, e.g., [19], p. 326). *Let $Z \in \mathcal{C}(\mathcal{H})$ and let $\lambda \in \sigma(Z)$ be isolated. If $P = P_Z(\lambda)$ is defined as above, then the following holds:*

(i) *P is a projection, i.e., $P^2 = P$.*
(ii) $\mathrm{Ran}(P)$ *and* $\mathrm{Ker}(P)$ *are Z-invariant.*
(iii) $\mathrm{Ran}(P) \subset \mathrm{Dom}(Z)$ *and* $Z|_{\mathrm{Ran}(P)}$ *is bounded.*
(iv) $\sigma(Z|_{\mathrm{Ran}(P)}) = \{\lambda\}$ *and* $\sigma(Z|_{\mathrm{Ker}(P)}) = \sigma(Z) \setminus \{\lambda\}$.

We say that $\lambda_0 \in \sigma(Z)$ is a discrete eigenvalue if λ_0 is an isolated point of $\sigma(Z)$ and $P = P_Z(\lambda_0)$ is of finite rank (in the literature these eigenvalues are also referred to as "eigenvalues of finite type"). Note that in this case λ_0 is indeed an eigenvalue of Z since $\{\lambda_0\} = \sigma(Z|_{\mathrm{Ran}(P)})$ and $\mathrm{Ran}(P)$ is Z-invariant and finite dimensional. The positive integer

$$m_Z(\lambda_0) := \mathrm{Rank}(P_Z(\lambda_0)) \tag{2.1.6}$$

is called the algebraic multiplicity of λ_0 with respect to Z. It has to be distinguished from the geometric multiplicity, which is defined as the dimension of the eigenspace $\mathrm{Ker}(\lambda_0 - Z)$ (and so can be smaller than the algebraic multiplicity).

Convention 2.1.2. *In this article only algebraic multiplicities will be considered and we will use the term "multiplicity" as a synonym for "algebraic multiplicity".*

The discrete spectrum of Z is now defined as

$$\sigma_d(Z) := \{\lambda \in \sigma(Z) : \lambda \text{ is a discrete eigenvalue of } Z\}. \tag{2.1.7}$$

We recall that a linear operator $Z_0 \in \mathcal{C}(\mathcal{H})$ is a Fredholm operator if it has closed range and both its kernel and cokernel are finite dimensional. Equivalently, if $Z_0 \in \mathcal{C}(\mathcal{H})$ is densely defined, then Z_0 is Fredholm if it has closed range and both $\mathrm{Ker}(Z_0)$ and $\mathrm{Ker}(Z_0^*)$ are finite dimensional. The essential spectrum of Z is defined as

$$\sigma_{\mathrm{ess}}(Z) := \{\lambda \in \mathbb{C} : \lambda - Z \text{ is not a Fredholm operator }\}.^4 \tag{2.1.8}$$

Note that $\sigma_{\mathrm{ess}}(Z) \subset \sigma(Z)$ and that $\sigma_{\mathrm{ess}}(Z)$ is a closed set.

For later purposes we will need the following result about the spectrum of the resolvent of Z.

Proposition 2.1.3 ([13], p. 243 and p. 247, and [8], p. 331). *Suppose that $Z \in \mathcal{C}(\mathcal{H})$ with $\rho(Z) \neq \emptyset$. If $a \in \rho(Z)$, then*

$$\sigma(R_Z(a)) \setminus \{0\} = \{(a - \lambda)^{-1} : \lambda \in \sigma(Z)\}.$$

[4] For a discussion of various alternative (non-equivalent) definitions of the essential spectrum we refer to [12]. We note that all reasonable definitions coincide in the selfadjoint case.

The same identity holds when, on both sides, σ is replaced by σ_{ess} and σ_d, respectively. More precisely, λ_0 is an isolated point of $\sigma(Z)$ if and only if $(a-\lambda_0)^{-1}$ is an isolated point of $\sigma(R_Z(a))$ and in this case

$$P_Z(\lambda_0) = P_{R_Z(a)}((a-\lambda_0)^{-1}).$$

In particular, the algebraic multiplicities of $\lambda_0 \in \sigma_d(Z)$ and $(a-\lambda_0)^{-1} \in \sigma_d(R_Z(a))$ coincide.

Remark 2.1.4. We note that $0 \in \sigma(R_Z(a))$ if and only if $Z \notin \mathcal{B}(\mathcal{H})$. Moreover, if $Z \in \mathcal{C}(\mathcal{H})$ is densely defined, then

$$0 \in \sigma(R_Z(a)) \quad \Leftrightarrow \quad 0 \in \sigma_{\mathrm{ess}}(R_Z(a)).$$

The following proposition shows that the essential and the discrete spectrum of a linear operator are disjoint.

Proposition 2.1.5. *If $Z \in \mathcal{C}(\mathcal{H})$ and λ is an isolated point of $\sigma(Z)$, then $\lambda \in \sigma_{\mathrm{ess}}(Z)$ if and only if* $\mathrm{Rank}(P_Z(\lambda)) = \infty$. *In particular,*

$$\sigma_{\mathrm{ess}}(Z) \cap \sigma_d(Z) = \emptyset.$$

Proof. For $Z \in \mathcal{B}(\mathcal{H})$ a proof can be found in [8], p. 122. The unbounded case can be reduced to the bounded case by means of Proposition 2.1.3. □

While the spectrum of a selfadjoint operator Z can always be decomposed as

$$\sigma(Z) = \sigma_{\mathrm{ess}}(Z) \,\dot{\cup}\, \sigma_d(Z), \tag{2.1.9}$$

where the symbol $\dot{\cup}$ denotes a disjoint union, the same need not be true in the non-selfadjoint case. For instance, considering the shift operator $(Zf)(n) = f(n+1)$ acting on $l^2(\mathbb{N})$, we have $\sigma_{\mathrm{ess}}(Z) = \{z \in \mathbb{C} : |z| = 1\}$ and $\sigma(Z) = \{z \in \mathbb{C} : |z| \leq 1\}$, while $\sigma_d(Z) = \emptyset$, see [33], pp. 237–238. The following result gives a suitable criterion for the discreteness of the spectrum in the complement of $\sigma_{\mathrm{ess}}(Z)$.

Proposition 2.1.6 ([19], p. 373). *Let $Z \in \mathcal{C}(\mathcal{H})$ and let $\Omega \subset \mathbb{C} \setminus \sigma_{\mathrm{ess}}(Z)$ be open and connected. If $\Omega \cap \rho(Z) \neq \emptyset$, then $\sigma(Z) \cap \Omega \subset \sigma_d(Z)$.*

Hence, if Ω is a (maximal connected) component of $\mathbb{C} \setminus \sigma_{\mathrm{ess}}(Z)$, then either

(i) $\Omega \subset \sigma(Z)$ (in particular, $\Omega \cap \sigma_d(Z) = \emptyset$), or
(ii) $\Omega \cap \rho(Z) \neq \emptyset$ and $\Omega \cap \sigma(Z)$ consists of an at most countable sequence of discrete eigenvalues which can accumulate at $\sigma_{\mathrm{ess}}(Z)$ only.

A direct consequence of Proposition 2.1.6 is

Corollary 2.1.7. *Let $Z \in \mathcal{C}(\mathcal{H})$ with $\sigma_{\mathrm{ess}}(Z) \subset \mathbb{R}$ and assume that there are points of $\rho(Z)$ in both the upper and lower half-planes. Then $\sigma(Z) = \sigma_{\mathrm{ess}}(Z) \,\dot{\cup}\, \sigma_d(Z)$.*

We conclude this section with some remarks on the numerical range of a linear operator and its relation to the spectrum, see [24], [33] for extensive accounts on this topic. The numerical range of $Z \in \mathcal{C}(\mathcal{H})$ is defined as

$$\mathrm{Num}(Z) := \{\langle Zf, f\rangle : f \in \mathrm{Dom}(Z), \|f\| = 1\}. \tag{2.1.10}$$

It was shown by Hausdorff and Toeplitz (see, e.g., [8] Theorem 9.3.1) that the numerical range is always a convex subset of $\mathbb{C}$. Furthermore, if the complement of the closure of the numerical range is connected and contains at least one point of the resolvent set of Z, then $\sigma(Z) \subset \overline{\mathrm{Num}}(Z)$ and

$$\|R_Z(a)\| \leq 1/\operatorname{dist}(a, \overline{\mathrm{Num}}(Z)), \qquad a \in \mathbb{C} \setminus \overline{\mathrm{Num}}(Z). \tag{2.1.11}$$

Clearly, if $Z \in \mathcal{B}(\mathcal{H})$ then $\mathrm{Num}(Z) \subset \{\lambda : |\lambda| \leq \|Z\|\}$. Moreover, if Z is normal then the closure of $\mathrm{Num}(Z)$ coincides with the convex hull of $\sigma(Z)$, i.e., the smallest convex set containing $\sigma(Z)$.

2.2. Schatten classes and determinants

An operator $K \in \mathcal{B}(\mathcal{H})$ is called compact if it is the norm limit of finite rank operators. The class of all compact operators forms a two-sided ideal in $\mathcal{B}(\mathcal{H})$, which we denote by $\mathcal{S}_\infty(\mathcal{H})$. The non-zero elements of the spectrum of $K \in \mathcal{S}_\infty(\mathcal{H})$ are discrete eigenvalues. In particular, the only possible accumulation point of the spectrum is 0, and 0 itself may or may not belong to the spectrum. More precisely, if $\mathcal{H}$ is infinite dimensional, as will be the case in most of the applications below, then $\sigma_{\mathrm{ess}}(K) = \{0\}$.

For every $K \in \mathcal{S}_\infty(\mathcal{H})$ we can find (not necessarily complete) orthonormal sets $\{\phi_n\}$ and $\{\psi_n\}$ in $\mathcal{H}$, and a set of positive numbers $\{s_n(K)\}$ with $s_1(K) \geq s_2(K) \geq \cdots > 0$, such that

$$Kf = \sum_n s_n(K)\langle f, \psi_n\rangle \phi_n, \qquad f \in \mathcal{H}. \tag{2.2.1}$$

Here the numbers $s_n(K)$ are called the singular values of K. They are precisely the eigenvalues of $|K| := \sqrt{K^*K}$, in non-increasing order.

The Schatten class of order p (with $p \in (0,\infty)$), denoted by $\mathcal{S}_p(\mathcal{H})$, consists of all compact operators on $\mathcal{H}$ whose singular values are p-summable, i.e.,

$$K \in \mathcal{S}_p(\mathcal{H}) \quad :\Leftrightarrow \quad \{s_n(K)\} \in l^p(\mathbb{N}). \tag{2.2.2}$$

We remark that $\mathcal{S}_p(\mathcal{H})$ is a linear subspace of $\mathcal{S}_\infty(\mathcal{H})$ for every $p > 0$ and for $p \geq 1$ we can make it into a complete normed space by setting

$$\|K\|_{\mathcal{S}_p} := \|\{s_n(K)\}\|_{l^p}. \tag{2.2.3}$$

Note that for $0 < p < 1$ this definition provides only a quasi-norm. For consistency we set $\|K\|_{S_\infty} := \|K\|$.

For $0 < p < q \leq \infty$ we have the (strict) inclusion $\mathcal{S}_p(\mathcal{H}) \subset \mathcal{S}_q(\mathcal{H})$ and

$$\|K\|_{\mathcal{S}_q} \leq \|K\|_{\mathcal{S}_p}. \tag{2.2.4}$$

Similar to the class of compact operators, $\mathcal{S}_p(\mathcal{H})$ is a two-sided ideal in the algebra $\mathcal{B}(\mathcal{H})$ and for $K \in \mathcal{S}_p(\mathcal{H})$ and $B \in \mathcal{B}(\mathcal{H})$ we have

$$\|KB\|_{\mathcal{S}_p} \leq \|K\|_{\mathcal{S}_p}\|B\| \quad \text{and} \quad \|BK\|_{\mathcal{S}_p} \leq \|B\|\|K\|_{\mathcal{S}_p}. \tag{2.2.5}$$

Moreover, if $K \in \mathcal{S}_p(\mathcal{H})$ then $K^* \in \mathcal{S}_p(\mathcal{H})$ and $\|K^*\|_{\mathcal{S}_p} = \|K\|_{\mathcal{S}_p}$.

The following estimate is a Schatten class analog of Hölder's inequality (see [20], p. 88): Let $K_1 \in \mathcal{S}_p(\mathcal{H})$ and $K_2 \in \mathcal{S}_q(\mathcal{H})$ where $0 < p, q \leq \infty$. Then $K_1K_2 \in \mathcal{S}_r(\mathcal{H})$, where $r^{-1} = p^{-1} + q^{-1}$, and

$$\|K_1K_2\|_{\mathcal{S}_r} \leq \|K_1\|_{\mathcal{S}_p}\|K_2\|_{\mathcal{S}_q}.$$

While the singular values of a selfadjoint operator are just the absolute values of its eigenvalues, in general the eigenvalues and singular values need not be related. However, we have the following result of Weyl.

Proposition 2.2.1. *Let $K \in \mathcal{S}_p(\mathcal{H})$, where $0 < p < \infty$, and let $\lambda_1, \lambda_2, \ldots$ denote its sequence of nonzero eigenvalues (counted according to their multiplicity). Then, for any $n \geq 1$*

$$\sum_{n=1}^{\infty} |\lambda_n|^p \leq \sum_{n=1}^{\infty} s_n(K)^p. \tag{2.2.6}$$

In the remaining part of this section we will introduce the notion of an infinite determinant. To this end, let $K \in \mathcal{S}_n(\mathcal{H})$, where $n \in \mathbb{N}$, and let $\lambda_1, \lambda_2, \ldots$ denote its sequence of nonzero eigenvalues, counted according to their multiplicity and enumerated according to decreasing absolute value. The n-regularized determinant of $I - K$, where I denotes the identity operator on $\mathcal{H}$, is

$$\det_n(I-K) := \begin{cases} \prod_{k\in\mathbb{N}}(1-\lambda_k), & \text{if } n = 1 \\ \prod_{k\in\mathbb{N}}\left[(1-\lambda_k)\exp\left(\sum_{j=1}^{n-1}\frac{\lambda_k^j}{j}\right)\right], & \text{if } n \geq 2. \end{cases} \tag{2.2.7}$$

Here the convergence of the products on the right-hand side follows from (2.2.6).

It is clear from the definition that $I - K$ is invertible if and only if $\det_n(I - K) \neq 0$. Moreover, $\det_n(I) = 1$. Since the nonzero eigenvalues of K_1K_2 and K_2K_1 coincide ($K_1, K_2 \in \mathcal{B}(\mathcal{H})$) we have

$$\det_n(I - K_1K_2) = \det_n(I - K_2K_1) \tag{2.2.8}$$

if both $K_1K_2, K_2K_1 \in \mathcal{S}_n(\mathcal{H})$.

The regularized determinant $\det_n(I - K)$ is a continuous function of K. If $\Omega \subset \hat{\mathbb{C}}$ is open and $K(\lambda) \in \mathcal{S}_n(\mathcal{H})$ is a family of operators which depends holomorphically on $\lambda \in \Omega$, then $\det_n(I - K(\lambda))$ is holomorphic on Ω. For a proof of both results we refer to [43].

We can define the perturbation determinant for non-integer-valued Schatten classes as well: Since $\mathcal{S}_p(\mathcal{H}) \subset \mathcal{S}_{\lceil p\rceil}(\mathcal{H})$ where $\lceil p\rceil = \min\{n \in \mathbb{N} : n \geq p\}$, the $\lceil p\rceil$-regularized determinant of $I - K, K \in \mathcal{S}_p(\mathcal{H})$, is well defined, and so the above results can still be applied. Moreover, this determinant can be estimated in terms of the pth Schatten norm of K (see [11], [43], [18]): If $K \in \mathcal{S}_p(\mathcal{H})$, where $0 < p < \infty$, then

$$|\det_{\lceil p\rceil}(I - K)| \leq \exp\left(\Gamma_p\|K\|_{\mathcal{S}_p}^p\right), \tag{2.2.9}$$

where Γ_p is some positive constant.

2.3. Perturbation theory

The aim of perturbation theory is to obtain information about the spectrum of some operator Z by showing that it is close, in a suitable sense, to an operator Z_0 whose spectrum is already known. In this case one can hope that some of the spectral characteristics of Z_0 are inherited by Z. For instance, the classical Weyl theorem (see Theorem 2.3.4 below) implies the validity of the following result (also sometimes called Weyl's Theorem).

Proposition 2.3.1. *Let $Z, Z_0 \in \mathcal{C}(\mathcal{H})$ with $\rho(Z) \cap \rho(Z_0) \neq \emptyset$. If the resolvent difference $R_Z(a) - R_{Z_0}(a)$ is compact for some $a \in \rho(Z) \cap \rho(Z_0)$, then $\sigma_{\text{ess}}(Z) = \sigma_{\text{ess}}(Z_0)$.*

Remark 2.3.2. If $R_Z(a) - R_{Z_0}(a)$ is compact for some $a \in \rho(Z) \cap \rho(Z_0)$, then the same is true for every $a \in \rho(Z) \cap \rho(Z_0)$. This is a consequence of the Hilbert identity

$$R_Z(b) - R_{Z_0}(b) = (a - Z)R_Z(b)(R_Z(a) - R_{Z_0}(a))(a - Z_0)R_{Z_0}(b),$$

valid for $a, b \in \rho(Z) \cap \rho(Z_0)$.

Combining Proposition 2.3.1 and Corollary 2.1.7 we obtain the following result for perturbations of selfadjoint operators.

Corollary 2.3.3. *Let $Z, Z_0 \in \mathcal{C}(\mathcal{H})$ and let Z_0 be selfadjoint. Suppose that there are points of $\rho(Z)$ in both the upper and lower half-planes. If $R_Z(a) - R_{Z_0}(a) \in \mathcal{S}_\infty(\mathcal{H})$ for some $a \in \rho(Z) \cap \rho(Z_0)$, then $\sigma_{\text{ess}}(Z) = \sigma_{\text{ess}}(Z_0) \subset \mathbb{R}$ and*

$$\sigma(Z) = \sigma_{\text{ess}}(Z_0) \,\dot{\cup}\, \sigma_d(Z). \tag{2.3.1}$$

In the following we will study perturbations of the form $Z = Z_0 + M$, understood as the usual operator sum defined on $\text{Dom}(Z_0) \cap \text{Dom}(M)$. More precisely, we assume that $Z_0 \in \mathcal{C}(\mathcal{H})$ has non-empty resolvent set and that M is a relatively bounded perturbation of Z_0, i.e., $\text{Dom}(Z_0) \subset \text{Dom}(M)$ and there exist $r, s \geq 0$ such that

$$\|Mf\| \leq r\|f\| + s\|Z_0 f\|$$

for all $f \in \text{Dom}(Z_0)$. The infimum of all constants s for which a corresponding r exists such that the last inequality holds is called the Z_0-bound of M. The operator Z is closed if the Z_0-bound of M is smaller than one. Note that M is Z_0-bounded if and only if $\text{Dom}(Z_0) \subset \text{Dom}(M)$ and $MR_{Z_0}(a) \in \mathcal{B}(\mathcal{H})$ for some $a \in \rho(Z_0)$, and the Z_0-bound is not larger than $\inf_{a \in \rho(Z_0)} \|MR_{Z_0}(a)\|$. The operator M is called Z_0-compact if $\text{Dom}(Z_0) \subset \text{Dom}(M)$ and $MR_{Z_0}(a) \in \mathcal{S}_\infty(\mathcal{H})$ for some $a \in \rho(Z_0)$. Every Z_0-compact operator is Z_0-bounded and the corresponding Z_0-bound is 0. Moreover, if M is Z_0-compact and Z_0 is Fredholm, then also $Z_0 + M$ is Fredholm (see, e.g., [33], p. 238). The last implication is the main ingredient in the proof of Weyl's theorem:

Theorem 2.3.4. *Let $Z = Z_0 + M$ where $Z_0 \in \mathcal{C}(\mathcal{H})$ and M is Z_0-compact. Then $\sigma_{\text{ess}}(Z) = \sigma_{\text{ess}}(Z_0)$.*

Remark 2.3.5. As noted above, Weyl's theorem and Proposition 2.1.3 show the validity of Proposition 2.3.1.

If Z_0 is selfadjoint and M is Z_0-compact, then $\rho(Z)$ has values in the upper and lower half-plane (see [8], p. 326). Moreover, if $a \in \rho(Z) \cap \rho(Z_0)$, then $R_Z(a) - R_{Z_0}(a) \in \mathcal{S}_\infty(\mathcal{H})$ as a consequence of the second resolvent identity

$$R_Z(a) - R_{Z_0}(a) = R_Z(a) M R_{Z_0}(a). \tag{2.3.2}$$

So Corollary 2.3.3 implies that $\sigma_{\text{ess}}(Z) = \sigma_{\text{ess}}(Z_0)$ and $\sigma(Z) = \sigma_{\text{ess}}(Z_0) \,\dot\cup\, \sigma_d(Z)$.

2.4. Perturbation determinants

We have seen in the last section that the essential spectrum is stable under (relatively) compact perturbations. In this section, we will have a look at the discrete spectrum and construct a holomorphic function whose zeros coincide with the discrete eigenvalues of the corresponding operator. Throughout we make the following assumption.

Assumption 2.4.1. *Z_0 and Z are closed densely defined operators in $\mathcal{H}$ such that*

(i) $\rho(Z_0) \cap \rho(Z) \neq \emptyset$.
(ii) $R_Z(b) - R_{Z_0}(b) \in \mathcal{S}_p(\mathcal{H})$ *for some* $b \in \rho(Z_0) \cap \rho(Z)$ *and some fixed* $p > 0$.
(iii) $\sigma(Z) \cap \rho(Z_0) = \sigma_d(Z)$.

Remark 2.4.2. By Proposition 2.3.3, assumption (iii) follows from assumption (ii) if Z_0 is selfadjoint with $\sigma_d(Z_0) = \emptyset$ and if there exist points of $\rho(Z)$ in both the upper and lower half-planes. If Z_0 and Z are bounded operators on $\mathcal{H}$ then the second resolvent identity implies that assumption (ii) is equivalent to $Z - Z_0 \in \mathcal{S}_p(\mathcal{H})$.

We begin with the case when $Z_0, Z \in \mathcal{B}(\mathcal{H})$: Then for $\lambda_0 \in \rho(Z_0)$ we have

$$(\lambda_0 - Z) R_{Z_0}(\lambda_0) = I - (Z - Z_0) R_{Z_0}(\lambda_0),$$

so $\lambda_0 \in \rho(Z)$ if and only if $I - (Z - Z_0) R_{Z_0}(\lambda_0)$ is invertible. As we know from Section 2.2, this operator is invertible if and only if

$$\det_{\lceil p \rceil}(I - (Z - Z_0) R_{Z_0}(\lambda_0)) \neq 0.$$

By Assumption 2.4.1 we have $\sigma(Z) \cap \rho(Z_0) = \sigma_d(Z)$, so we have shown that $\lambda_0 \in \sigma_d(Z)$ if and only if λ_0 is a zero of the analytic function

$$d_\infty^{Z,Z_0} : \hat\rho(Z_0) \to \mathbb{C}, \qquad d_\infty^{Z,Z_0}(\lambda) := \det_{\lceil p \rceil}(I - (Z - Z_0) R_{Z_0}(\lambda)). \tag{2.4.1}$$

For later purposes we note that $d_\infty^{Z,Z_0}(\infty) = 1$.

Next, we consider the general case: Let $a \in \rho(Z_0) \cap \rho(Z)$ where Z_0, Z satisfy Assumption 2.4.1. Then Proposition 2.1.3 and its accompanying remark show that

$$\sigma_d(R_Z(a)) = \sigma(R_Z(a)) \cap \rho(R_{Z_0}(a)),$$

so we can apply the previous discussion to the operators $R_{Z_0}(a)$ and $R_Z(a)$, i.e., the function

$$d_\infty^{R_Z(a), R_{Z_0}(a)}(.) = \det_{\lceil p \rceil}(I - [R_Z(a) - R_{Z_0}(a)][(.) - R_{Z_0}(a)]^{-1}) \tag{2.4.2}$$

is well defined and analytic on $\hat{\rho}(R_{Z_0}(a))$. Moreover, since $\lambda \in \hat{\rho}(Z_0)$ if and only if $(a-\lambda)^{-1} \in \hat{\rho}(R_{Z_0}(a))$ (which is again a consequence of Proposition 2.1.3 and Remark 2.1.4), we see that the function

$$d_a^{Z,Z_0}(\lambda) := d_\infty^{R_Z(a),R_{Z_0}(a)}((a-\lambda)^{-1}) \tag{2.4.3}$$

is analytic on $\hat{\rho}(Z_0)$ and

$$d_a^{Z,Z_0}(\lambda) = 0 \quad \Leftrightarrow \quad (a-\lambda)^{-1} \in \sigma_d(R_Z(a)) \quad \Leftrightarrow \quad \lambda \in \sigma_d(Z).$$

Note that, as above, we have $d_a^{Z,Z_0}(a) = d_\infty^{R_Z(a),R_{Z_0}(a)}(\infty) = 1$.

We summarize the previous discussion in the following proposition.

Proposition 2.4.3. *Let $a \in \hat{\rho}(Z_0) \cap \hat{\rho}(Z)$, where Z, Z_0 satisfy Assumption* 2.4.1*, and let $d_a = d_a^{Z,Z_0} : \hat{\rho}(Z_0) \to \mathbb{C}$ be defined by* (2.4.1) *if $a = \infty$ and by* (2.4.3) *if $a \neq \infty$, respectively. Then d_a is analytic, $d_a(a) = 1$ and $\lambda \in \sigma_d(Z)$ if and only if $d_a(\lambda) = 0$.*

We call the function $d_a = d_a^{Z,Z_0}$ the pth perturbation determinant of Z by Z_0 (the p-dependence of d_a is neglected in our notation). Without proof we note that the algebraic multiplicity of $\lambda_0 \in \sigma_d(Z)$ coincides with the order of λ_0 as a zero of d_a, see [25], pp. 20–22.

Remark 2.4.4. Our definition of perturbation determinants is an extension of the standard one (which coincides with the function d_∞), see, e.g., [21] and [45].

We conclude this section with some estimates.

Proposition 2.4.5. *Let $a \in \rho(Z_0) \cap \rho(Z)$, where Z, Z_0 satisfy Assumption* 2.4.1*, and let $d_a : \hat{\rho}(Z_0) \to \mathbb{C}$ be defined as above. Then, for $\lambda \neq a$,*

$$|d_a(\lambda)| \leq \exp\left(\Gamma_p \|[R_Z(a) - R_{Z_0}(a)][(a-\lambda)^{-1} - R_{Z_0}(a)]^{-1}\|_{\mathcal{S}_p}^p\right), \tag{2.4.4}$$

where Γ_p was introduced in estimate (2.2.9)*.*

Proof. Apply estimate (2.2.9). □

Proposition 2.4.6. *Let $Z, Z_0 \in \mathcal{B}(\mathcal{H})$ satisfy Assumption* 2.4.1*. Then for $\lambda \in \hat{\rho}(Z_0)$ we have*

$$|d_\infty(\lambda)| \leq \exp\left(\Gamma_p \|(Z - Z_0)R_{Z_0}(\lambda)\|_{\mathcal{S}_p}^p\right). \tag{2.4.5}$$

If, in addition, $Z - Z_0 = M_1 M_2$ where M_1, M_2 are bounded operators on $\mathcal{H}$ such that $M_2 R_{Z_0}(a) M_1 \in \mathcal{S}_p(\mathcal{H})$ for every $a \in \rho(Z_0)$, then for $\lambda \in \hat{\rho}(Z_0)$ we have

$$|d_\infty(\lambda)| \leq \exp\left(\Gamma_p \|M_2 R_{Z_0}(\lambda) M_1\|_{\mathcal{S}_p}^p\right). \tag{2.4.6}$$

Proof. Estimate (2.4.6) is a consequence of estimate (2.2.9), the definition of d_∞ and the identity

$$\det_{\lceil p \rceil}(I - (Z - Z_0)R_{Z_0}(\lambda)) = \det_{\lceil p \rceil}(I - M_1 M_2 R_{Z_0}(\lambda)) = \det_{\lceil p \rceil}(I - M_2 R_{Z_0}(\lambda) M_1),$$

which follows from (2.2.8). Estimate (2.4.5) follows immediately from the definition of d_∞ and estimate (2.2.9). □

Remark 2.4.7. While the non-zero eigenvalues of $M_1M_2R_{Z_0}(a)$ and $M_2R_{Z_0}(a)M_1$ coincide, the same need not be true for their singular values. In particular, while $(Z - Z_0)R_{Z_0}(a) \in \mathcal{S}_p(\mathcal{H})$ is automatically satisfied if $Z, Z_0 \in \mathcal{B}(\mathcal{H})$ satisfy Assumption 2.4.1, in general this need not imply that $M_2R_{Z_0}(a)M_1 \in \mathcal{S}_p(\mathcal{H})$ as well.

3. Zeros of holomorphic functions

In this chapter we discuss results on the distribution of zeros of holomorphic functions, which will subsequently be applied to the holomorphic functions defined by perturbation determinants to obtain results on the distribution of eigenvalues for certain classes of operators. We begin with a motivating discussion in Section 3.1, introducing the class of functions on the unit disk which will be our special focus of study. In Section 3.2 we consider results that can be obtained using the classical Jensen identity. In Section 3.3 we present the recent results of Borichev, Golinskii and Kupin and show that, for the class of functions that we are interested in, they yield more information than provided by the application of the Jensen identity.

3.1. Motivation: the complex analysis method for studying eigenvalues

We have seen in Section 2.4 that the discrete spectrum of a linear operator Z satisfying Assumption 2.4.1 coincides with the zero set of the corresponding perturbation determinant, which is a holomorphic function defined on the resolvent set of the 'unperturbed' operator Z_0. Moreover, we have a bound on the absolute value of this holomorphic function in the form of Propositions 2.4.5 and 2.4.6. Thus, general results providing information about the zeros of holomorphic functions satisfying certain bounds may be exploited to obtain information about the eigenvalues of the operator Z. This observation is the basis of the following complex-analysis approach to studying eigenvalues.

As an example, we consider the following situation: $Z_0 \in \mathcal{B}(\mathcal{H})$ is assumed to be a selfadjoint operator with

$$\sigma(Z_0) = \sigma_{\text{ess}}(Z_0) = [a, b], \tag{3.1.1}$$

where $a < b$, and

$$Z = Z_0 + M,$$

where $M \in \mathcal{S}_p(\mathcal{H})$ for some fixed $p > 0$. Given these assumptions, the spectrum of Z can differ from the spectrum of Z_0 by an at most countable set of discrete eigenvalues, whose points of accumulation are contained in the interval $[a, b]$. Moreover, $\sigma_d(Z)$ is precisely the zero set of the pth perturbation determinant $d = d_\infty^{Z,Z_0}$ defined by

$$d : \hat{\mathbb{C}} \setminus [a, b] \to \mathbb{C}, \qquad d(\lambda) = \det{}_{\lceil p \rceil}(I - MR_{Z_0}(\lambda)).$$

It should therefore be possible to obtain further information on the distribution of the eigenvalues of Z by studying the analytic function d, in particular, by taking advantage of the estimate provided on d in Proposition 2.4.6, i.e.,

$$\log|d(\lambda)| \leq \Gamma_p \|MR_{Z_0}(\lambda)\|_{\mathcal{S}_p}^p, \qquad \lambda \in \mathbb{C} \setminus [a,b], \tag{3.1.2}$$

as well as the fact that $d(\infty) = 1$. Note that the right-hand side of (3.1.2) is finite for any $\lambda \in \hat{\mathbb{C}} \setminus [a,b]$, but as λ approaches $[a,b]$ it can 'explode'. A simple way to estimate the right-hand side of (3.1.2) from above and thus to obtain a more concrete estimate, is to use the identity

$$\|R_{Z_0}(\lambda)\| = [\mathrm{dist}(\lambda, \sigma(Z_0))]^{-1}, \tag{3.1.3}$$

which is valid since Z_0 is selfadjoint, and the inequality (2.2.5) to obtain

$$\log|d(\lambda)| \leq \frac{\Gamma_p \|M\|_{\mathcal{S}_p}^p}{\mathrm{dist}(\lambda, \sigma(Z_0))^p}. \tag{3.1.4}$$

The inequality (3.1.4) is the best that we can obtain at a general level, that is without imposing any further restrictions on the operators Z_0 and M. However, as we shall show in Chapter 7.1, for concrete operators it is possible to obtain better inequalities by a more precise analysis of the $\mathcal{S}_p$-norm of $MR_{Z_0}(\lambda)$. These inequalities will take the general form

$$\log|d(\lambda)| \leq \frac{C}{\mathrm{dist}(\lambda, \sigma(Z_0))^{\alpha'} \, \mathrm{dist}(\lambda, a)^{\beta_1'} \, \mathrm{dist}(\lambda, b)^{\beta_2'}}, \tag{3.1.5}$$

where α' and β_1', β_2' are some non-negative parameters with $\alpha' + \beta_1' + \beta_2' = p$. Note that (3.1.5) can be stronger than (3.1.4) in the sense that the growth of $\log|d(\lambda)|$ as λ approaches a point $\zeta \in (a,b)$ is estimated from above by $O(|\lambda - \zeta|^{-\alpha'})$, which can be smaller than the $O(|\lambda - \zeta|^{-p})$ bound given by (3.1.4) (since $\alpha' < p$ if $\beta_1' + \beta_2' > 0$). A similar remark applies to λ approaching one of the endpoints a, b (since, e.g., $\alpha' + \beta_1' < p$ if $\beta_2' > 0$). As we shall see, such differences are very significant in terms of the estimates on eigenvalues that are obtained.

The question then becomes how to use inequalities of the type (3.1.4), (3.1.5) to deduce information about the zeros of the holomorphic function $d(.)$. The study of zeros of holomorphic functions is, of course, a major theme in complex analysis. Since the holomorphic functions $d(.)$ which we will be looking at will be defined on domains that are conformally equivalent to the open unit disk $\mathbb{D}$, we are specifically interested in results about zeros of functions $h \in H(\mathbb{D})$, the class of holomorphic functions in the unit disk. Indeed, if $\Omega \subset \hat{\mathbb{C}}$ is a domain which is conformally equivalent to the unit disk, we choose a conformal map $\phi : \mathbb{D} \to \Omega$ so that the study of the zeros of the holomorphic function $d : \Omega \to \mathbb{C}$ is converted to the study of the zeros of the function $h = d \circ \phi : \mathbb{D} \to \mathbb{C}$, where, denoting by $\mathcal{Z}(h)$ the set of zeros of a holomorphic function h, we have

$$\mathcal{Z}(d|_\Omega) = \phi(\mathcal{Z}(h)).$$

If $\infty \in \Omega$, we can also choose the conformal mapping ϕ so that $\phi(0) = \infty$, which implies that $h(0) = 1$.

This conversion involves two steps which require some effort:

(i) Inequalities of the type (3.1.4) and (3.1.5) must be translated into inequalities on the function $h \in H(\mathbb{D})$.

(ii) Results obtained about the zeros of h, lying in the unit disk, must be translated into results about the zeros of d.

Regarding step (i), it turns out that inequalities of the form (3.1.5), and generalizations of it, are converted into inequalities of the form

$$\log|h(w)| \leq \frac{K|w|^{\gamma}}{(1-|w|)^{\alpha} \prod_{j=1}^{N} |w-\xi_j|^{\beta_j}}, \quad w \in \mathbb{D}, \tag{3.1.6}$$

where $\xi_j \in \mathbb{T} := \partial\mathbb{D}$ and the parameters in (3.1.6) are determined by those appearing in the inequality bounding $d(\lambda)$ and by properties of the conformal mapping ϕ. Note that this inequality restricts the growth of $|h(w)|$ as $|w| \to 1$ differently according to whether or not w approaches one of the 'special' points ξ_j. Since functions obeying (3.1.6) play an important role in our work, it is convenient to have a special notation for this class of functions. First, let us set

$$(\mathbb{T}^N)_* := \{(\xi_1, \ldots, \xi_N) \in \mathbb{T}^N : \xi_i \neq \xi_j, 1 \leq i < j \leq N\}, \quad N \in \mathbb{N}. \tag{3.1.7}$$

Definition 3.1.1. Let $\alpha, \gamma, K \in \mathbb{R}_+ := [0, \infty)$. For $N \in \mathbb{N}$ let $\vec{\beta} = (\beta_1, \ldots, \beta_N) \in \mathbb{R}_+^N$ and $\vec{\xi} = (\xi_1, \ldots, \xi_N) \in (\mathbb{T}^N)_*$. The class of all functions $h \in H(\mathbb{D})$ satisfying $h(0) = 1$ and obeying (3.1.6) (for this choice of parameters) is denoted by $\mathcal{M}(\alpha, \vec{\beta}, \gamma, \vec{\xi}, K)$. Moreover, we set $\mathcal{M}(\alpha, K) = \mathcal{M}(\alpha, \vec{0}, 0, \vec{\xi}, K)$ where $\vec{\xi} \in \mathbb{T}^N$ is arbitrary, that is functions satisfying

$$\log|h(w)| \leq \frac{K}{(1-|w|)^{\alpha}}, \quad w \in \mathbb{D}.$$

Remark 3.1.2. Throughout this chapter, whenever speaking of $\mathcal{M}(\alpha, \vec{\beta}, \gamma, \vec{\xi}, K)$ we will always implicitly assume that the parameters are chosen as indicated in the previous definition.

Remark 3.1.3. We have the inclusions

$$\mathcal{M}(\alpha, \vec{\beta}, \gamma, \vec{\xi}, K) \subset \mathcal{M}(\alpha', \vec{\beta}, \gamma', \vec{\xi}, K')$$

if $\alpha \leq \alpha', \gamma \geq \gamma'$ and $K \leq K'$, and

$$\mathcal{M}(\alpha, \vec{\beta}, \gamma, \vec{\xi}, K) \subset \mathcal{M}(\alpha, \vec{\beta}', \gamma, \vec{\xi}, K \cdot 2^{\sum_{j=1}^{N} \beta_j'})$$

if $\beta_j \leq \beta_j'$ for $1 \leq j \leq N$.

Thus, our aim is to understand what information on the set of zeros of h is implied by the assumption $h \in \mathcal{M}(\alpha, \vec{\beta}, \gamma, \vec{\xi}, K)$. This information will then be translated back into information about the set of zeros of the perturbation determinant $d(\lambda)$, that is about the eigenvalues of Z.

3.2. Zeros of holomorphic functions in the unit disk: Jensen's identity

The zero set of a (non-trivial) function $h \in H(\mathbb{D})$ is of course discrete, with possible accumulation points on the boundary $\mathbb{T}$. In other words, $\mathcal{Z}(h)$ is either finite, or it can be written as $\mathcal{Z}(h) = \{w_k\}_{k=1}^{\infty}$, where $|w_k|$ is increasing, and

$$\lim_{k \to \infty} (1 - |w_k|) = 0. \tag{3.2.1}$$

While in this generality nothing more can be said about $\mathcal{Z}(h)$, the situation changes drastically if we restrict the growth of $|h(z)|$ as z approaches the boundary of the unit disk. A basic result which allows to make a connection between the boundary growth of a function $h \in H(\mathbb{D})$ and the distribution of its zeros is Jensen's identity (see [40], p. 308). Denoting the number of zeros (counting multiplicities) of h in the disk $\mathbb{D}_r = \{w \in \mathbb{C} : |w| \leq r\}$ by $N(h,r)$, this result reads as follows.

Lemma 3.2.1. *Let $h \in H(\mathbb{D})$ with $|h(0)| = 1$. Then for $r \in (0,1)$ we have*

$$\int_0^r \frac{N(h,s)}{s}\, ds = \sum_{w \in \mathcal{Z}(h), |w| \leq r} \log\left|\frac{r}{w}\right| = \frac{1}{2\pi}\int_0^{2\pi} \log|h(re^{i\theta})|\, d\theta. \tag{3.2.2}$$

Note that the left equality is immediate, while the right equality is the real content of the result.

As a simple application of Jensen's identity, consider the case in which $h \in H^{\infty}(\mathbb{D})$, the class of functions bounded in the unit disk, with $\|h\|_{\infty}$ denoting the supremum. Then the right-hand side of (3.2.2) is bounded from above by $\log(\|h\|_{\infty})$, so that we can take the limit $r \to 1-$ (noting that the left-hand side increases with r) and obtain

$$\sum_{w \in \mathcal{Z}(h)} \log\left|\frac{1}{w}\right| \leq \log(\|h\|_{\infty}).$$

We may also bound the left-hand side of this inequality from below, using $\log|w| \leq |w| - 1$, to obtain

$$\sum_{w \in \mathcal{Z}(h)} (1 - |w|) \leq \log(\|h\|_{\infty}). \tag{3.2.3}$$

Obviously the convergence of the sum in (3.2.3), known as the Blaschke sum, is a much stricter condition on the sequence of zeros than (3.2.1). However, the functions h arising in the applications we make to the perturbation determinant will generally not be bounded, so the Blaschke condition (3.2.3) cannot be applied. We will now assume that $h \in \mathcal{M} = \mathcal{M}(\alpha, \vec{\beta}, \gamma, \vec{\xi}, K)$ and derive estimates on the zeros of h, by using Jensen's identity in a more careful way.

We will use the following proposition, derived from Jensen's identity. For that purpose we denote the *support* of a function $f : (a,b) \subset \mathbb{R} \to \mathbb{R}$ by $\mathrm{supp}(f)$, i.e.,

$$\mathrm{supp}(f) = \overline{\{x \in (a,b) : f(x) \neq 0\}}.$$

Moreover, by $f_+ = \max(f,0)$ and $f_- = -\min(f,0)$ we denote the positive and negative parts of f, respectively (note that we will use the same notation for the positive and negative parts of a real number as well). In addition, we denote the class of all twice-differentiable functions on (a, b) whose second derivative is continuous by $C^2(a, b)$.

Proposition 3.2.2. *Let $\varphi \in C^2(0,1)$ be non-negative and non-increasing, and suppose that* $\lim_{r\to 1}\varphi(r) = \lim_{r\to 1}\varphi'(r) = 0$, $\operatorname{supp}([r\varphi'(r)]')_- \subset [0,1)$ *and*

$$\sup_{0<r<1}([r\varphi'(r)]')_- < \infty.$$

If $h \in H(\mathbb{D})$, with $|h(0)| = 1$, then

$$\sum_{w\in\mathcal{Z}(h)} \varphi(|w|) = \frac{1}{2\pi}\int_0^1 dr\,[r\varphi'(r)]' \int_0^{2\pi} d\theta \log|h(re^{i\theta})|.^5 \qquad (3.2.4)$$

Remark 3.2.3. We are mainly interested in the choice $\varphi(r) = (1-r)^q$, with $q > 1$; other possible choices are $\varphi(r) = (-\log(r))^q$ and $\varphi(r) = (r^{-1}-r)^q$, respectively.

Proof of Proposition 3.2.2. Let $0 < r < 1$. We restate Jensen's identity:

$$\int_0^r ds\,\frac{N(h,s)}{s} = \frac{1}{2\pi}\int_0^{2\pi} d\theta \log|h(re^{i\theta})|. \qquad (3.2.5)$$

Multiplying both sides of (3.2.5) by $[r\varphi'(r)]'$ and integrating with respect to r leads to

$$\begin{aligned}
&\frac{1}{2\pi}\int_0^1 dr\,[r\varphi'(r)]' \int_0^{2\pi} d\theta\ \log|h(re^{i\theta})| \\
&= \int_0^1 dr\,[r\varphi'(r)]' \int_0^r ds\,\frac{N(h,s)}{s} \overset{(\star)}{=} \int_0^1 ds\,\frac{N(h,s)}{s}\int_s^1 dr\,[r\varphi'(r)]' \\
&= -\int_0^1 ds\,\varphi'(s)N(h,s) = \int_0^\infty dt\,\left[\frac{d}{dt}\varphi(e^{-t})\right] N(h,e^{-t}).
\end{aligned} \qquad (3.2.6)$$

The application of Fubini's theorem in $(\star)$ is justified by the assumptions made on φ. We can reformulate the right-hand side of the last equation as follows

$$\begin{aligned}
&\int_0^\infty dt\,\left[\frac{d}{dt}\varphi(e^{-t})\right] N(h,e^{-t}) = \int_0^\infty dt \sum_{w\in\mathcal{Z}(h),|w|<e^{-t}} \left[\frac{d}{dt}\varphi(e^{-t})\right] \\
&= \sum_{w\in\mathcal{Z}(h)} \int_0^{-\log|w|} dt\,\left[\frac{d}{dt}\varphi(e^{-t})\right] = \sum_{w\in\mathcal{Z}(h)} \varphi(|w|).
\end{aligned}$$

The last equation together with (3.2.6) yields the result. □

We can now derive a Blaschke-type result on the zeros of a function $h \in \mathcal{M}$ (see Definition 3.1.1). In the result below, $C(\alpha, \vec{\beta}, \vec{\xi}, \tau)$ denotes a constant depending only on the parameters $\alpha, \vec{\beta}, \vec{\xi}, \tau$, which can in principle be made explicit but would yield expressions too unwieldy to be of much use. As usual, when such a constant appears in two equations, or even on two lines of the same equations, it

[5] Of course, both sides of (3.2.4) may be (simultaneously) divergent.

may take different values, but we do take care to always indicate the parameters on which the constant depends.

Theorem 3.2.4. *Let $h \in \mathcal{M}(\alpha, \vec{\beta}, 0, \vec{\xi}, K)$. Then for every $\tau > 0$ we have*

$$\sum_{w \in \mathcal{Z}(h)} (1-|w|)^{1+\alpha+\max_j(\beta_j-1)_+ +\tau} \leq C(\alpha, \vec{\beta}, \vec{\xi}, \tau) K. \tag{3.2.7}$$

Proof. For $q > 1$ let $\varphi(r) = (1-r)^q$. Since

$$[r\varphi'(r)]' = q(1-r)^{q-2}(rq-1)$$

we obtain from Proposition 3.2.2 and our assumptions, using that $\int\limits_0^{2\pi} \log|h(re^{i\theta})| d\theta$ is non-negative,

$$\begin{aligned}
\sum_{w \in \mathcal{Z}(h)} (1-|w|)^q &= \frac{q}{2\pi} \int_0^1 dr \frac{(rq-1)}{(1-r)^{2-q}} \int_0^{2\pi} d\theta \log|h(re^{i\theta})| \\
&\leq \frac{q}{2\pi} \int_{1/q}^1 dr \frac{(rq-1)}{(1-r)^{2-q}} \int_0^{2\pi} d\theta \, \log|h(re^{i\theta})| \\
&\leq \frac{Kq(q-1)}{2\pi} \int_{1/q}^1 dr \frac{1}{(1-r)^{2-q+\alpha}} \int_0^{2\pi} \frac{d\theta}{\prod_{j=1}^N |re^{i\theta}-\xi_j|^{\beta_j}} \\
&\leq \frac{KC(\vec{\beta}, \vec{\xi}) q(q-1)}{2\pi} \sum_{j=1}^N \int_{1/q}^1 dr \frac{1}{(1-r)^{2-q+\alpha}} \int_0^{2\pi} \frac{d\theta}{|re^{i\theta}-\xi_j|^{\beta_j}}.
\end{aligned} \tag{3.2.8}$$

Standard calculations show that, as $r \to 1-$

$$\int_0^{2\pi} \frac{d\theta}{|re^{i\theta}-\xi|^\beta} = \begin{cases} O\left(\frac{1}{(1-r)^{\beta-1}}\right), & \text{if } \beta > 1, \\ O\left(-\log(1-r)\right), & \text{if } \beta = 1, \\ O(1), & \text{if } \beta < 1. \end{cases} \tag{3.2.9}$$

Therefore the integrals on the right-hand side of (3.2.8) will be finite whenever $q > 1 + \alpha + \max_j(\beta_j - 1)_+$, and the result follows. □

3.3. A theorem of Borichev, Golinskii and Kupin

A different inequality on the zeros of $h \in \mathcal{M}(\alpha, \vec{\beta}, 0, \vec{\xi}, K)$ was proved by Borichev, Golinskii and Kupin [5].

Theorem 3.3.1. *Let $h \in \mathcal{M}(\alpha, \vec{\beta}, 0, \vec{\xi}, K)$, where $\vec{\xi} = (\xi_1, \ldots, \xi_N) \in (\mathbb{T}^N)_*$ and $\vec{\beta} = (\beta_1, \ldots, \beta_N) \in \mathbb{R}_+^N$. Then for every $\tau > 0$ the following holds: If $\alpha > 0$ then*

$$\sum_{w \in \mathcal{Z}(h)} (1-|w|)^{\alpha+1+\tau} \prod_{j=1}^N |w-\xi_j|^{(\beta_j-1+\tau)_+} \leq C(\alpha, \vec{\beta}, \vec{\xi}, \tau) K. \tag{3.3.1}$$

Furthermore, if $\alpha = 0$ *then*

$$\sum_{w\in\mathcal{Z}(h)}(1-|w|)\prod_{j=1}^{N}|w-\xi_j|^{(\beta_j-1+\tau)_+} \le C(\vec{\beta},\vec{\xi},\tau)K. \tag{3.3.2}$$

To see the advantage of (3.3.1) over (3.2.7), consider a convergent subsequence $\{w_k\}_{k=1}^{\infty} \subset \mathcal{Z}(h)$. The limit point ξ satisfies $|\xi| = 1$, and (3.2.7) ensures that the sum

$$\sum_{k=1}^{\infty}(1-|w_k|)^{\eta} < \infty \tag{3.3.3}$$

whenever

$$\eta > 1 + \alpha + \max_j(\beta_j - 1)_+. \tag{3.3.4}$$

As for (3.3.1), it gives us different information according to whether $\xi = \xi_j$ for some $1 \le j \le N$ or whether $\xi \in \partial\mathbb{D}$ is a 'generic' point. For sequences $\{w_k\}_{k=1}^{\infty}$ converging to generic points ($\xi \neq \xi_j$) the product term in (3.3.1) will be bounded from below by a positive constant along the sequence, so that we can conclude that (3.3.3) will hold whenever $\eta > \alpha + 1$, obviously a less restrictive condition than that provided by (3.3.4), except in the case when $\beta_j \le 1$ for all j, in which the two conditions are the same. When $\xi = \xi_{j^*}$ for some $1 \le j^* \le N$, the summands in (3.3.1) will be bounded from below by a positive constant multiple of

$$(1-|w_k|)^{\alpha+1+\tau}|w_k - \xi_{j^*}|^{(\beta_{j^*}-1+\tau)_+} \ge (1-|w_k|)^{\alpha+1+\tau+(\beta_{j^*}-1+\tau)_+}.$$

Therefore, if $\beta_{j^*} > 1$, (3.3.1) implies that (3.3.3) will hold whenever $\eta > \alpha+1+\beta_{j^*}$, a less restrictive condition than (3.3.4) since it does not involve the maximum of all β_j's. If $\beta_{j^*} < 1$, (3.3.1) implies that (3.3.3) will hold whenever $\eta > \alpha + 1$, also a less restrictive condition except in the case where all $\beta_j < 1$ for all $1 \le j \le N$, in which it is the same condition.

We thus see that the theorem of Borichev, Golinskii and Kupin [5] provides sharper information about the asymptotic distribution of the zeros than Theorem 3.2.4. Therefore, in our applications, Theorem 3.3.1 will provide more precise information about the distribution of eigenvalues, and it is this result which will be used. It should be noted that, unlike Theorem 3.2.4, the proof of Theorem 3.3.1 is not an application of Jensen's identity, and requires less elementary function-theoretic arguments.

Remark 3.3.2. We should also note that Theorem 3.3.1 has been generalized in several ways: to subharmonic functions on the unit disk [14], and to holomorphic functions on more general domains [23], [15]. We will return to this topic in Chapter 8.

In the following, however, we will make one improvement to Theorem 3.3.1, which is useful when considering applications to eigenvalue estimates. We consider functions $h \in \mathcal{M}(\alpha,\vec{\beta},\gamma,\vec{\xi},K)$ with $\gamma > 0$, which have the property that

$$\log|h(w)| = O(|w|^{\gamma}), \quad \text{as } |w| \to 0.$$

Of course these functions are included in $\mathcal{M}(\alpha, \vec{\beta}, 0, \vec{\xi}, K)$, so that Theorem 3.3.1 holds for them. We will show that, for this class of functions, the sum on the left-hand side of (3.3.1) can be replaced by

$$\sum_{w \in \mathcal{Z}(h)} \frac{(1-|w|)^{\alpha+1+\tau}}{|w|^x} \prod_{j=1}^{N} |w-\xi_j|^{(\beta_j-1+\tau)_+} \tag{3.3.5}$$

for a suitable choice of $x = x(\gamma) > 0$. It should be noted that since we always assume $h(0) = 1$, the zeros of h will always be bounded away from 0, so that (3.3.1) implies that the sum (3.3.5) is finite. The point, however, is to obtain a bound on this sum which is linear in K, like the bound in Theorem 3.3.1. This linearity is important in the applications.

We first estimate the counting function $N(h,r)$ for small $r > 0$.

Lemma 3.3.3. *Let $h \in \mathcal{M}(\alpha, \vec{\beta}, \gamma, \vec{\xi}, K)$. Then for $r \in (0, \frac{1}{2}]$ we have*

$$N(h,r) \leq C(\alpha, \vec{\beta}, \vec{\xi}) K r^{\gamma}. \tag{3.3.6}$$

Proof. Let $0 < r < s < 1$. Then,

$$N(h,r) = \frac{1}{\log(\frac{s}{r})} \int_r^s \frac{N(h,r)}{t} dt \leq \frac{1}{\log(\frac{s}{r})} \int_r^s \frac{N(h,t)}{t} dt \leq \frac{1}{\log(\frac{s}{r})} \int_0^s \frac{N(h,t)}{t} dt.$$

Jensen's identity and our assumptions on h thus imply that

$$\begin{aligned} N(h,r) &\leq \frac{1}{\log(\frac{s}{r})} \frac{1}{2\pi} \int_0^{2\pi} \log|h(se^{i\theta})| d\theta \\ &\leq \frac{1}{\log(\frac{s}{r})} \frac{K s^{\gamma}}{(1-s)^{\alpha}} \frac{1}{2\pi} \int_0^{2\pi} \prod_{j=1}^{N} \frac{1}{|se^{i\theta}-\xi_j|^{\beta_j}} d\theta. \end{aligned}$$

Choosing $s = \frac{3}{2} r$ (i.e., $s \leq \frac{3}{4}$) concludes the proof. □

The information offered by the previous lemma can immediately be applied to obtain the following result.

Lemma 3.3.4. *Let $h \in \mathcal{M}(\alpha, \vec{\beta}, \gamma, \vec{\xi}, K)$. Then for every $\varepsilon > 0$ we have*

$$\sum_{w \in \mathcal{Z}(h), |w| \leq \frac{1}{2}} \frac{1}{|w|^{(\gamma-\varepsilon)_+}} \leq C(\alpha, \vec{\beta}, \gamma, \vec{\xi}, \varepsilon) K. \tag{3.3.7}$$

Proof. For $\gamma \leq \varepsilon$ the left-hand side of (3.3.7) is equal to $N(h, 1/2)$, so in view of Lemma 3.3.3 we only need to consider the case $\gamma > \varepsilon$. In this case, we can rewrite the sum in (3.3.7) as follows:

$$\begin{aligned} \sum_{\substack{w \in \mathcal{Z}(h) \\ |w| \leq \frac{1}{2}}} \frac{1}{|w|^{\gamma-\varepsilon}} &= (\gamma-\varepsilon) \sum_{\substack{w \in \mathcal{Z}(h) \\ |w| \leq \frac{1}{2}}} \int_0^{\frac{1}{|w|}} dt\, t^{\gamma-1-\varepsilon} \\ &= (\gamma-\varepsilon) \left[\int_0^2 dt\, t^{\gamma-1-\varepsilon} N(h,1/2) + \int_2^{\infty} dt\, t^{\gamma-1-\varepsilon} N(h,t^{-1}) \right]. \end{aligned}$$

Using Lemma 3.3.3 and the fact that $\gamma > \varepsilon$ we conclude that

$$\int_0^2 dt\, t^{\gamma-1-\varepsilon} N(h,1/2) \le C(\alpha,\vec{\beta},\gamma,\vec{\xi},\varepsilon)K.$$

Similarly, using that $\varepsilon > 0$, Lemma 3.3.3 implies that

$$\begin{aligned}\int_2^\infty dt\, t^{\gamma-1-\varepsilon} N(h,t^{-1}) &\le C(\alpha,\vec{\beta},\vec{\xi})K \int_2^\infty dt\, t^{-1-\varepsilon}\\ &\le C(\alpha,\vec{\beta},\gamma,\vec{\xi},\varepsilon)K.\end{aligned}$$

This concludes the proof. □

The next theorem (which first appeared in [28]) combines the previous lemma with Theorem 3.2.4 to provide the desired bound on the sum in (3.3.5).

Theorem 3.3.5. *Let $h \in \mathcal{M}(\alpha,\vec{\beta},\gamma,\vec{\xi},K)$, where $\vec{\xi} = (\xi_1,\ldots,\xi_N) \in (\mathbb{T}^N)_*$ and $\vec{\beta} = (\beta_1,\ldots,\beta_N) \in \mathbb{R}_+^N$. Then for every $\varepsilon,\tau > 0$ the following holds: If $\alpha > 0$ then*

$$\sum_{w\in\mathcal{Z}(h)} \frac{(1-|w|)^{\alpha+1+\tau}}{|w|^{(\gamma-\varepsilon)_+}} \prod_{j=1}^N |w-\xi_j|^{(\beta_j-1+\tau)_+} \le C(\alpha,\vec{\beta},\gamma,\vec{\xi},\varepsilon,\tau)K. \tag{3.3.8}$$

Furthermore, if $\alpha = 0$ then

$$\sum_{w\in\mathcal{Z}(h)} \frac{(1-|w|)}{|w|^{(\gamma-\varepsilon)_+}} \prod_{j=1}^N |w-\xi_j|^{(\beta_j-1+\tau)_+} \le C(\vec{\beta},\gamma,\vec{\xi},\varepsilon,\tau)K. \tag{3.3.9}$$

Proof. Since the sum on the left-hand side of (3.3.8) is bounded from above by

$$\sum_{w\in\mathcal{Z}(h),|w|\le\frac{1}{2}} \frac{1}{|w|^{(\gamma-\varepsilon)_+}} + C(\gamma,\varepsilon) \sum_{w\in\mathcal{Z}(h),|w|>\frac{1}{2}} (1-|w|)^{\alpha+1+\tau} \prod_{j=1}^N |w-\xi_j|^{(\beta_j-1+\tau)_+},$$

we see that the proof of (3.3.8) is an immediate consequence of estimate (3.3.1) and Lemma 3.3.4. The proof of (3.3.9) is analogous starting from estimate (3.3.2). □

4. Eigenvalue estimates via the complex analysis approach

Applying the results obtained in the previous two chapters we derive estimates on the discrete spectrum of linear operators satisfying Assumption 2.4.1. In particular, we present precise estimates on the discrete spectrum of perturbations of bounded and non-negative selfadjoint operators, respectively. Some of the material in this section is taken from [25].

4.1. Bounded operators – a general result

Throughout this section we make the following

Assumption 4.1.1. *Z_0 and Z are bounded operators in $\mathcal{H}$, satisfying*

(i) *$M = Z - Z_0 \in \mathcal{S}_p(\mathcal{H})$ for some $p > 0$.*
(ii) *$\sigma_d(Z) = \sigma(Z) \cap \rho(Z_0)$.*
(iii) *M_1 and M_2 are two fixed bounded operators on $\mathcal{H}$ such that $M = M_1 M_2$ and $M_2 R_{Z_0}(a) M_1 \in \mathcal{S}_p(\mathcal{H})$ for every $a \in \hat{\rho}(Z_0)$.*
(iv) *$\hat{\rho}(Z_0)$ is conformally equivalent to the unit disk, that is there exists a (necessarily unique) mapping $\phi : \mathbb{D} \to \hat{\rho}(Z_0)$ with $\phi(0) = \infty$.*

Remark 4.1.2. We note that, if assumption (i) holds, assumption (iii) will automatically hold if we take $M_1 = I, M_2 = M$. However, sometimes other factorizations of M will yield stronger results, and for an arbitrary factorization $M = M_1 M_2$ it is not true that (i) implies (iii).

As we have seen in Section 2.4, the perturbation determinant

$$d = d_\infty^{Z,Z_0} : \hat{\rho}(Z_0) \to \mathbb{C}, \qquad d_\infty^{Z,Z_0}(\lambda) = \det_{\lceil p \rceil}(I - (Z - Z_0) R_{Z_0}(\lambda))$$

has the property that its zero set coincides with the discrete spectrum of Z, and $d(\infty) = 1$. We recall that, by (2.2.8),

$$\det_{\lceil p \rceil}(I - (Z - Z_0) R_{Z_0}(\lambda)) = \det_{\lceil p \rceil}(I - M_2 R_{Z_0}(\lambda) M_1),$$

and estimate (2.4.6) showed that for $\lambda \in \hat{\rho}(Z_0)$ we have

$$|d(\lambda)| \leq \exp\left(\Gamma_p \|M_2 R_{Z_0}(\lambda) M_1\|_{\mathcal{S}_p}^p\right), \tag{4.1.1}$$

where the constant Γ_p was introduced in (2.2.9). Thus if we can show that, for suitable parameters $\gamma, K, \alpha, \xi_j, \beta_j$,

$$\|M_2 R_{Z_0}(\phi(w)) M_1\|_{\mathcal{S}_p}^p \leq \frac{K|w|^\gamma}{(1-|w|)^\alpha \prod_{j=1}^N |w - \xi_j|^{\beta_j}}, \quad w \in \mathbb{D}, \tag{4.1.2}$$

then we obtain

$$\log|(d \circ \phi)(w)| \leq \frac{\Gamma_p K |w|^\gamma}{(1-|w|)^\alpha \prod_{j=1}^N |w - \xi_j|^{\beta_j}}.$$

In other words, $d \circ \phi \in \mathcal{M}(\alpha, \vec{\beta}, \gamma, \vec{\xi}, \Gamma_p K)$. Therefore Theorem 3.3.5 can be applied to $d \circ \phi$ and in this way we obtain the following result.

Proposition 4.1.3. *Suppose* (4.1.2) *holds, where $\alpha, \beta_j, \gamma, K$ are non-negative and $\xi_j \in \mathbb{T}$ are pairwise distinct. Then for every $\varepsilon, \tau > 0$ the following holds: If $\alpha > 0$ then*

$$\sum_{\lambda \in \sigma_d(Z)} \frac{(1 - |\phi^{-1}(\lambda)|)^{\alpha+1+\tau}}{|\phi^{-1}(\lambda)|^{(\gamma-\varepsilon)_+}} \prod_{j=1}^N |\phi^{-1}(\lambda) - \xi_j|^{(\beta_j - 1 + \tau)_+} \leq CK, \tag{4.1.3}$$

where $C = C(\alpha, \vec{\beta}, \gamma, \vec{\xi}, \varepsilon, \tau, p)$ *and each eigenvalue is counted according to its multiplicity. Moreover, if* $\alpha = 0$ *then the same inequality holds with* $\alpha + 1 + \tau$ *replaced by* 1*.*

Remark 4.1.4. It remains an interesting open question whether (4.1.3) is still valid when $\tau = 0$ and $\varepsilon = 0$, respectively. At the moment, even for the specific choices of Z_0 considered below, we are neither able to answer the corresponding question in the affirmative nor to provide a suitable counterexample.

Convention 4.1.5. *In the remaining parts of this article, let us agree that whenever a sum involving eigenvalues is considered, each eigenvalue is counted according to its* (*algebraic*) *multiplicity.*

The previous result is very general but not very enlightening. To obtain useful information using Proposition 4.1.3 we need to do two things:

- Obtain estimates of the form (4.1.2) for the operator of interest.
- Obtain estimates from below on the sum on the left-hand side of (4.1.3) in terms of simple functions of the eigenvalues, so as to obtain interesting information on the eigenvalues.

Carrying out both of these steps requires us to impose restrictions on the spectrum of the unperturbed operator Z_0, thus enabling us to express the mapping ϕ explicitly. In the next subsection we will concentrate on the case that Z_0 is self-adjoint, so that its spectrum is real. There are, however, various other options for treating various classes of operators. We now demonstrate one of them.

Example 4.1.6. Let $Z_0 \in \mathcal{B}(\mathcal{H})$ be normal. Assume that $\sigma(Z_0) = \sigma_{\text{ess}}(Z_0) = \overline{\mathbb{D}}$, and let $Z = Z_0 + M$ where $M \in \mathcal{S}_p(\mathcal{H})$ (so with the notation above we have $Z - Z_0 = M_1 M_2$, where $M_1 = I$ and $M_2 = M$). Note that $\sigma_d(Z) = \sigma(Z) \cap \overline{\mathbb{D}}^c$ by Proposition 2.1.6. A conformal map $\phi : \mathbb{D} \to \hat{\rho}(Z_0)$, mapping 0 onto ∞, is given by $\phi(w) = w^{-1}$, and we have $M_2 R_{Z_0}(w^{-1}) M_1 = M R_{Z_0}(w^{-1})$. The spectral theorem for normal operators implies that

$$\|R_{Z_0}(w^{-1})\| = \text{dist}(w^{-1}, \mathbb{T})^{-1} = |w|(1 - |w|)^{-1},$$

so we obtain

$$\|M R_{Z_0}(\phi(w))\|_{\mathcal{S}_p}^p \leq \|M\|_{\mathcal{S}_p}^p |w|^p (1 - |w|)^{-p}, \quad w \in \mathbb{D}.$$

Hence, applying Proposition 4.1.3 with $\alpha = \gamma = p$, $\vec{\beta} = \vec{0}$ and $K = \|M\|_{\mathcal{S}_p}^p$, we conclude that for $\tau \in (0, p)$ (choosing $\varepsilon = \tau$)

$$\sum_{\lambda \in \sigma_d(Z)} \frac{(|\lambda| - 1)^{p+1+\tau}}{|\lambda|^{1+2\tau}} = \sum_{\lambda \in \sigma_d(Z)} \frac{(1 - |\phi^{-1}(\lambda)|)^{p+1+\tau}}{|\phi^{-1}(\lambda)|^{p-\tau}} \leq C(p, \tau) \|M\|_{\mathcal{S}_p}^p.$$

Remark 4.1.7. Actually, we will show below that the estimate in the previous example can be improved considerably using our alternative approach to eigenvalue estimates (see Example 5.2.4).

4.2. Perturbations of bounded selfadjoint operators

Throughout this section we assume that $A_0 \in \mathcal{B}(\mathcal{H})$ is selfadjoint with $\sigma(A_0) = [a,b]$,[6] where $a < b$, and that $M = M_1 M_2 \in \mathcal{S}_p(\mathcal{H})$ for some $p > 0$, where M_1 and M_2 are bounded operators on $\mathcal{H}$ satisfying

$$M_2 R_{A_0}(\lambda) M_1 \in \mathcal{S}_p(\mathcal{H}), \quad \lambda \in \hat{\rho}(A_0). \tag{4.2.1}$$

In particular, A_0 and $A = A_0 + M$ satisfy Assumption 2.4.1 by Remark 2.4.2 (with $Z_0 = A_0$ and $Z = A$, respectively), and we have

$$\sigma(A) = [a,b] \,\dot{\cup}\, \sigma_d(A).$$

Let us define a conformal map $\phi_1 : \mathbb{D} \to \hat{\mathbb{C}} \setminus [a,b]$, mapping 0 onto ∞, by setting

$$\phi_1(w) = \frac{b-a}{4}(w + w^{-1} + 2) + a, \quad w \in \mathbb{D}. \tag{4.2.2}$$

To adapt Proposition 4.1.3 to the present context we will need the following elementary but crucial inequalities, see Lemma 7 in [28].

Lemma 4.2.1. *For $w \in \mathbb{D}$ let $\phi_1(w)$ be defined by* (4.2.2). *Then*

$$\frac{b-a}{8}\frac{|w^2-1|(1-|w|)}{|w|} \leq \operatorname{dist}(\phi_1(w),[a,b]) \leq \frac{(b-a)(1+\sqrt{2})}{8}\frac{|w^2-1|(1-|w|)}{|w|}.$$

In the following, we derive estimates on $\sigma_d(A)$ given the assumption that for every $\lambda \in \mathbb{C} \setminus [a,b]$ we have

$$\|M_2 R_{A_0}(\lambda) M_1\|_{\mathcal{S}_p}^p \leq K \frac{|\lambda-a|^\beta |\lambda-b|^\beta}{\operatorname{dist}(\lambda,[a,b])^\alpha}, \tag{4.2.3}$$

where $\alpha, K \in \mathbb{R}_+$, $\beta \in \mathbb{R}$ and $\alpha > 2\beta$. Of course, one could imagine different assumptions on the norm of $M_2 R_{A_0}(\lambda) M_1$, e.g., a different behavior at the boundary points a and b, but the choice above is sufficiently general for the applications we have in mind.

Theorem 4.2.2. *With the assumptions and notations from above, suppose that $M_2 R_{A_0}(\lambda) M_1$ satisfies estimate* (4.2.3) *for every $\lambda \in \mathbb{C} \setminus [a,b]$. Let $\tau \in (0,1)$ and define*

$$\begin{aligned} \eta_1 &= \alpha + 1 + \tau, \\ \eta_2 &= (\alpha - 2\beta - 1 + \tau)_+. \end{aligned} \tag{4.2.4}$$

Then the following holds: If $\alpha > 0$ then

$$\sum_{\lambda \in \sigma_d(A)} \frac{\operatorname{dist}(\lambda,[a,b])^{\eta_1}}{(|b-\lambda||a-\lambda|)^{\frac{\eta_1-\eta_2}{2}}} \leq C(\alpha,\beta,\tau,p)(b-a)^{\eta_2-\alpha+2\beta} K. \tag{4.2.5}$$

Moreover, if $\alpha = 0$ then the same inequality holds with η_1 replaced by 1.

[6] In this section we are changing notation from Z_0 to A_0 (and from Z to A), the reason being the specific choice we make for the spectrum of A_0. A similar remark will apply in Section 4.4.

Proof. We consider the case $\alpha > 0$ only. As above, let

$$\lambda = \phi_1(w) = \frac{b-a}{4}(w + w^{-1} + 2) + a, \qquad w \in \mathbb{D}.$$

Then a short computation shows that

$$|a - \lambda| = \frac{b-a}{4}\frac{|w+1|^2}{|w|} \quad \text{and} \quad |b - \lambda| = \frac{b-a}{4}\frac{|w-1|^2}{|w|}. \tag{4.2.6}$$

Using the last two identities and Lemma 4.2.1, the assumption in (4.2.3) can be rewritten as

$$\|M_2 R_{A_0}(\lambda) M_1\|_{\mathcal{S}_p}^p \leq \frac{C(\alpha,\beta)K}{(b-a)^{\alpha-2\beta}} \frac{|w|^{\alpha-2\beta}}{(1-|w|)^{\alpha}|w^2-1|^{\alpha-2\beta}}. \tag{4.2.7}$$

Let $\varepsilon, \tau > 0$ and let η_1, η_2 be defined by (4.2.4). Then Proposition 4.1.3 implies that

$$\sum_{\lambda \in \sigma_d(A)} \frac{(1-|\phi_1^{-1}(\lambda)|)^{\eta_1}}{|\phi_1^{-1}(\lambda)|^{(\alpha-2\beta-\varepsilon)_+}} |(\phi_1^{-1}(\lambda))^2 - 1|^{\eta_2} \leq \frac{C(\alpha,\beta,\varepsilon,\tau,p)K}{(b-a)^{\alpha-2\beta}}. \tag{4.2.8}$$

Restricting τ to the interval $(0,1)$ and setting $\varepsilon = 1 - \tau$, the last inequality can be rewritten as

$$\sum_{\lambda \in \sigma_d(A)} \frac{(1-|\phi_1^{-1}(\lambda)|)^{\eta_1}}{|\phi_1^{-1}(\lambda)|^{\eta_2}} |(\phi_1^{-1}(\lambda))^2 - 1|^{\eta_2} \leq \frac{C(\alpha,\beta,\tau,p)K}{(b-a)^{\alpha-2\beta}}. \tag{4.2.9}$$

By (4.2.6) we have

$$|(\phi_1^{-1}(\lambda))^2 - 1| = \frac{4}{b-a}|\phi_1^{-1}(\lambda)|(|\lambda - a||\lambda - b|)^{1/2}, \tag{4.2.10}$$

and by Lemma 4.2.1, we obtain

$$\begin{aligned}(1 - |\phi_1^{-1}(\lambda)|) &\geq \frac{8}{(1+\sqrt{2})(b-a)} \frac{|\phi_1^{-1}(\lambda)| \operatorname{dist}(\lambda,[a,b])}{|(\phi_1^{-1}(\lambda))^2 - 1|} \\ &= \frac{2}{(1+\sqrt{2})} \frac{\operatorname{dist}(\lambda,[a,b])}{(|\lambda-a||\lambda-b|)^{1/2}}. \end{aligned} \tag{4.2.11}$$

Inserting (4.2.11) and (4.2.10) into (4.2.9) concludes the proof. □

Remark 4.2.3. The left- and right-hand sides of (4.2.11) are actually equivalent (meaning that the same inequality, with another constant, holds in the other direction as well), so no essential information gets lost in this estimate.

Remark 4.2.4. A nice way to illustrate the consequences of the finiteness of the sum in (4.2.5) is to consider sequences $\{\lambda_k\}$ of isolated eigenvalues of A converging to some $\lambda^* \in [a,b]$. Taking a subsequence, we can suppose that one of the following options holds:

(i.a) $\lambda^* = a$ and $\mathrm{Re}(\lambda_k) \leq a$. (i.b) $\lambda^* = b$ and $\mathrm{Re}(\lambda_k) \geq b$.

(ii.a) $\lambda^* = a$ and $\mathrm{Re}(\lambda_k) > a$. (ii.b) $\lambda^* = b$ and $\mathrm{Re}(\lambda_k) < b$.

(iii) $\lambda^* \in (a,b)$.

It is sufficient to consider the cases (i.a), (ii.a) and (iii) only. In case (i.a), since $\operatorname{dist}(\lambda_k, [a,b]) = |\lambda_k - a|$, (4.2.5) implies the finiteness of $\sum_k |\lambda_k - a|^{(\eta_1+\eta_2)/2}$ showing that any such sequence must converge to a sufficiently fast. Similarly, in case (ii.a), (4.2.5) implies the finiteness of $\sum_k \frac{|\operatorname{Im}(\lambda_k)|^{\eta_1}}{|\lambda_k - a|^{(\eta_1-\eta_2)/2}}$. Finally, in case (iii), we obtain the finiteness of $\sum_k |\operatorname{Im}(\lambda_k)|^{\eta_1}$, showing that the sequence must converge to the real line sufficiently fast.

Theorem 4.2.2 still relies on a quantitative estimate on the $\mathcal{S}_p$-norm of the operator $M_2 R_{A_0}(\lambda) M_1$. In particular applications, one wants to choose the decomposition $M = M_1 M_2$ so as to obtain an estimate on $M_2 R_{A_0}(\lambda) M_1$ as strong as possible (we will indicate this process when considering Jacobi operators in Chapter 7.1). Let us note, however, that we can always take the 'trivial' decomposition $M_1 = I$ and $M_2 = M$, and use the bound

$$\|M R_{A_0}(\lambda)\|_{\mathcal{S}_p}^p \leq \|M\|_{\mathcal{S}_p}^p \|R_{A_0}(\lambda)\|^p \leq \frac{\|M\|_{\mathcal{S}_p}^p}{\operatorname{dist}(\lambda, [a,b])^p},$$

so that we obtain the following estimates.

Corollary 4.2.5. *Let $A_0 \in \mathcal{B}(\mathcal{H})$ be selfadjoint with $\sigma(A_0) = [a,b]$ and let $A = A_0 + M$ where $M \in \mathcal{S}_p(\mathcal{H})$. Then for $\tau \in (0,1)$ the following holds: If $p \geq 1 - \tau$ then*

$$\sum_{\lambda \in \sigma_d(A)} \frac{\operatorname{dist}(\lambda, [a,b])^{p+1+\tau}}{|b-\lambda||a-\lambda|} \leq C(p,\tau)(b-a)^{-1+\tau} \|M\|_{\mathcal{S}_p}^p. \tag{4.2.12}$$

Moreover, if $0 < p < 1 - \tau$ then

$$\sum_{\lambda \in \sigma_d(A)} \left(\frac{\operatorname{dist}(\lambda, [a,b])}{|b-\lambda|^{1/2}|a-\lambda|^{1/2}} \right)^{p+1+\tau} \leq C(p,\tau)(b-a)^{-p} \|M\|_{\mathcal{S}_p}^p. \tag{4.2.13}$$

Proof. Apply Theorem 4.2.2 with $M_1 = I$, $M_2 = M$, $K = \|M\|_{\mathcal{S}_p}^p$, $\alpha = p$ and $\beta = 0$. □

Remark 4.2.6. In view of estimate (4.2.13), we should mention that in general it is not possible to infer the finiteness of the sum

$$\sum_{\lambda \in \sigma_d(A_0+M)} \left(\frac{\operatorname{dist}(\lambda, [a,b])}{|b-\lambda|^{1/2}|a-\lambda|^{1/2}} \right)^{\gamma}, \quad \text{where } \gamma < 1, \tag{4.2.14}$$

from the mere assumption that $M \in \mathcal{S}_p(\mathcal{H})$ for some $p > 0$. Indeed, if A_0 is the free Jacobi operator, then for every $\gamma < 1$ we can construct a rank one perturbation M such that the sum in (4.2.14) diverges, see Appendix C in [25].

Remark 4.2.7. We note that a slightly weaker version of the previous theorem has first been obtained by Borichev, Golinskii and Kupin [5] in the context of Jacobi operators. They used Theorem 3.3.1 instead of Theorem 3.3.5 in its derivation, which resulted in a constant on the right-hand side depending on the operator A in some unspecified way.

We will return to Corollary 4.2.5 in Chapter 6, where we will compare it with some related results obtained via our alternative approach to eigenvalue estimates, which will be described in Chapter 5.

4.3. Unbounded operators – a general result

We are now interested in applying similar considerations to the study of eigenvalues of unbounded operators. Throughout this section we make the following

Assumption 4.3.1. *Z_0 and Z are operators in $\mathcal{H}$ satisfying*

(i) *$Z, Z_0 \in \mathcal{C}(\mathcal{H})$ are densely defined with $\rho(Z_0) \cap \rho(Z) \neq \emptyset$.*
(ii) *$R_Z(b) - R_{Z_0}(b) \in \mathcal{S}_p(\mathcal{H})$ for some $b \in \rho(Z_0) \cap \rho(Z)$ and some $p > 0$.*
(iii) *$\sigma_d(Z) = \sigma(Z) \cap \rho(Z_0)$.*
(iv) *$\rho(Z_0)$ is conformally equivalent to the unit disk. More precisely, there exists a conformal mapping $\psi : \mathbb{D} \to \rho(Z_0)$ with $\psi(0) = a$, where a is some fixed element of $\rho(Z_0) \cap \rho(Z)$.*

The analysis of the discrete spectrum of Z is quite similar to the analysis made in Section 4.1, with the only difference that the discrete spectrum of Z now coincides with the zero set of the perturbation determinant

$$d_a^{Z,Z_0} : \rho(Z_0) \to \mathbb{C}, \quad d_a^{Z,Z_0}(\lambda) = \det_{\lceil p \rceil}(I - [R_Z(a) - R_{Z_0}(a)][(a-\lambda)^{-1} - R_{Z_0}(a)]^{-1}),$$

compare Section 2.4. In particular, we can use the same line of reasoning as in Section 4.1 to obtain the following result.

Proposition 4.3.2. *Suppose that for some non-negative constants $K, \alpha, \beta_j, \gamma$ and some pairwise distinct $\xi_j \in \mathbb{T}$ we have for every $w \in \mathbb{D}$*

$$\|[R_Z(a) - R_{Z_0}(a)][(a - \psi(w))^{-1} - R_{Z_0}(a)]^{-1}\|_{\mathcal{S}_p}^p \leq \frac{K|w|^\gamma}{(1-|w|)^\alpha \prod_{j=1}^N |w - \xi_j|^{\beta_j}}. \quad (4.3.1)$$

Then for every $\varepsilon, \tau > 0$ the following holds: If $\alpha > 0$ then

$$\sum_{\lambda \in \sigma_d(Z)} \frac{(1 - |\psi^{-1}(\lambda)|)^{\alpha+1+\tau}}{|\psi^{-1}(\lambda)|^{(\gamma-\varepsilon)_+}} \prod_{j=1}^N |\psi^{-1}(\lambda) - \xi_j|^{(\beta_j - 1 + \tau)_+} \leq C(\alpha, \vec{\beta}, \gamma, \vec{\xi}, \varepsilon, \tau, p) K.$$

Moreover, if $\alpha = 0$ then the same inequality holds with $\alpha + 1 + \tau$ replaced by 1.

Remark 4.3.3. If $Z = Z_0 + M$ where M is Z_0-compact, then we can use the second resolvent identity (2.3.2) to obtain

$$[R_Z(a) - R_{Z_0}(a)][(a - \psi(w))^{-1} - R_{Z_0}(a)]^{-1} = (a - \psi(w)) R_Z(a) M R_{Z_0}(\psi(w)),$$

so in order to satisfy the conditions of the last proposition we need a good control of the $\mathcal{S}_p$-norm of $MR_{Z_0}(\psi(w))$. We will return to this topic in the next section.

We can obtain a more "explicit" version of Proposition 4.3.2 using Koebe's distortion theorem, see [39], page 9.

Theorem 4.3.4. *Let $\varphi : \mathbb{D} \to \varphi(\mathbb{D})$ be conformal. Then*

$$\frac{1}{4}|\varphi'(w)|(1-|w|) \leq \operatorname{dist}(\varphi(w), \partial\varphi(\mathbb{D})) \leq 2|\varphi'(w)|(1-|w|) \tag{4.3.2}$$

for $w \in \mathbb{D}$.

Corollary 4.3.5. *Suppose that* (4.3.1) *is satisfied for some non-negative constants $K, \alpha, \beta_j, \gamma$ and some pairwise distinct $\xi_j \in \mathbb{T}$. Then for every $\varepsilon, \tau > 0$ the following holds: If $\alpha > 0$ then*

$$\sum_{\lambda \in \sigma_d(Z)} \frac{(\operatorname{dist}(\lambda, \partial\sigma(Z_0))|(\psi^{-1})'(\lambda)|)^{\alpha+1+\tau}}{|\psi^{-1}(\lambda)|^{(\gamma-\varepsilon)_+}} \prod_{j=1}^{N} |\psi^{-1}(\lambda) - \xi_j|^{(\beta_j-1+\tau)_+} \leq CK, \tag{4.3.3}$$

where $C = C(\alpha, \vec{\beta}, \gamma, \vec{\xi}, \varepsilon, \tau, p)$. Moreover, if $\alpha = 0$ then the same inequality holds with $\alpha + 1 + \tau$ replaced by 1.

Proof. Use Proposition 4.3.2 and the fact that, by Koebe's distortion theorem, for $\lambda \in \rho(Z_0) = \psi(\mathbb{D})$ we have

$$4 \operatorname{dist}(\lambda, \partial\rho(Z_0)) \geq (1 - |\psi^{-1}(\lambda)|)|\psi'(\psi^{-1}(\lambda))| \geq \frac{1}{2} \operatorname{dist}(\lambda, \partial\rho(Z_0)).$$

Now note that $\partial\rho(Z_0) = \partial\sigma(Z_0)$. □

4.4. Perturbations of non-negative operators

In this section we assume that H_0 is a selfadjoint operator in $\mathcal{H}$ with $\sigma(H_0) = [0, \infty)$, and $H \in \mathcal{C}(\mathcal{H})$ is densely defined with

$$R_H(u) - R_{H_0}(u) \in \mathcal{S}_p(\mathcal{H}) \tag{4.4.1}$$

for some $u \in \rho(H_0) \cap \rho(H)$ (which we assume to be non-empty) and some fixed $p \in (0, \infty)$. In particular, by Remark 2.4.2, H_0 and H satisfy Assumption 2.4.1 (with $Z_0 = H_0$ and $Z = H$, respectively) and we have

$$\sigma(H) = [0, \infty) \,\dot{\cup}\, \sigma_d(H).$$

Remark 4.4.1. Given the above assumptions we could use Corollary 4.3.5 to derive a quite explicit estimate on the discrete eigenvalues of H in terms of the $\mathcal{S}_p$-norm of $R_H(u) - R_{H_0}(u)$, see [25] Theorem 3.3.1. However, we decided against presenting this estimate in this review since it is weaker than an analogous estimate we can obtain using our alternative approach to eigenvalue estimates (see Theorem 5.3.1).

Actually, in the following we will restrict ourselves to a less general but much simpler situation: We will assume that $H = H_0 + M$ where M is H_0-compact and $MR_{H_0}(u) \in \mathcal{S}_p(\mathcal{H})$ for some (and hence all) $u \in \rho(H_0)$. Moreover, we will assume that there exists $\omega \leq 0$ such that

$$\{\lambda : \operatorname{Re}(\lambda) < \omega\} \subset \rho(H) \tag{4.4.2}$$

and that there exists $C_0(\omega) > 0$ such that for every λ with $\operatorname{Re}(\lambda) < \omega$ we have

$$\|R_H(\lambda)\| \leq \frac{C_0(\omega)}{|\operatorname{Re}(\lambda) - \omega|}. \tag{4.4.3}$$

Remark 4.4.2. The existence of some ω with the above properties is actually implied by the H_0-compactness of M (see, e.g., the discussion in [25] Section 3.3). If the operator H is m-sectorial with vertex $\gamma \leq 0$, then we can choose $\omega = \gamma$ and $C_0(\omega) = 1$. For instance, the Schrödinger operators considered in Chapter 7.2 will be m-sectorial.

Now let us fix some $a < \omega$ and choose $b > 0$ such that $a = -b^2$. For later purposes let us note that a conformal mapping ψ_1 of $\mathbb{D}$ onto $\mathbb{C} \setminus [0, \infty)$, which maps 0 onto a, is given by

$$\psi_1(w) = a\left(\frac{1+w}{1-w}\right)^2, \quad \psi_1^{-1}(\lambda) = \frac{\sqrt{-\lambda} - b}{\sqrt{-\lambda} + b}. \tag{4.4.4}$$

Here the square root is chosen such that $\mathrm{Re}(\sqrt{-\lambda}) > 0$ for $\lambda \in \mathbb{C} \setminus [0, \infty)$. In particular, we note that $\psi_1(-1) = 0$ and $\psi_1(1) = \infty$.

In the following, we will derive a first estimate on $\sigma_d(H)$ (which will not use estimate (4.4.3)) given the quantitative assumption that for every $\lambda \in \mathbb{C} \setminus [0, \infty)$ we have

$$\|R_H(a)MR_{H_0}(\lambda)\|_{\mathcal{S}_p}^p \leq \frac{K|\lambda|^\beta}{\mathrm{dist}(\lambda, [0, \infty))^\alpha}, \tag{4.4.5}$$

where α, K are non-negative and $\beta \in \mathbb{R}$ (note that the values of the constants might also depend on the choice of a).

Theorem 4.4.3. *With the assumptions and notation from above, assume that the operator $R_H(a)MR_{H_0}(\lambda)$ satisfies assumption* (4.4.5)*. Let $\varepsilon, \tau > 0$ and define*

$$\begin{aligned} \eta_1 &= \alpha + 1 + \tau, \\ \eta_2 &= ((\alpha - 2\beta)_+ - 1 + \tau)_+, \\ \eta_3 &= ((2p - 3\alpha + 2\beta)_+ - 1 + \tau)_+, \\ \eta_4 &= (p - \varepsilon)_+. \end{aligned} \tag{4.4.6}$$

Then the following holds: If $\alpha > 0$ then

$$\sum_{\lambda \in \sigma_d(H)} \frac{\mathrm{dist}(\lambda, [0, \infty))^{\eta_1}}{|\lambda|^{\frac{\eta_1 - \eta_2}{2}} (|\lambda| + |a|)^{\eta_1 - \eta_4 + \frac{\eta_2 + \eta_3}{2}} |\lambda - a|^{\eta_4}} \leq C|a|^{-(\frac{\eta_1 + \eta_3}{2} - p + \alpha - \beta)} K, \tag{4.4.7}$$

where $C = C(\alpha, \beta, p, \varepsilon, \tau)$. Furthermore, if $\alpha = 0$ then the same inequality holds with η_1 replaced by 1*.*

Remark 4.4.4. The parameter $\frac{\eta_1 + \eta_3}{2} - p + \alpha - \beta$ is positive, as a short computation shows.

Proof of Theorem 4.4.3. We consider the case $\alpha > 0$ only. Let $\lambda = \psi_1(w) = a(\frac{1+w}{1-w})^2$ and note that

$$\psi_1(w) - a = \frac{4aw}{(1-w)^2}.$$

Together with assumption (4.4.5), the last identity implies that

$$|\psi_1(w) - a|^p \|R_H(a)MR_{H_0}(\psi_1(w))\|_{\mathcal{S}_p}^p \leq \frac{4^p|a|^p|w|^p}{|1-w|^{2p}} \frac{K|\psi_1(w)|^\beta}{\mathrm{dist}(\psi_1(w), [0, \infty))^\alpha}. \tag{4.4.8}$$

Since $\psi_1'(w) = \frac{4a(1+w)}{(1-w)^3}$, we obtain from Theorem 4.3.4 that

$$\operatorname{dist}(\psi_1(w), [0,\infty)) \geq |a| \frac{|1+w|(1-|w|)}{|1-w|^3}.$$

Using this inequality and the definition of ψ_1 we see that the right-hand side of (4.4.8) is bounded from above by

$$\frac{4^p K |a|^{p-\alpha+\beta} |w|^p}{(1-|w|)^\alpha |1+w|^{\alpha-2\beta} |1-w|^{2p-3\alpha+2\beta}}.$$

Applying Corollary 4.3.5, taking Remark 4.3.3 into account, we thus obtain that for $\varepsilon, \tau > 0$,

$$\sum_{\lambda \in \sigma_d(H)} \frac{|\operatorname{dist}(\lambda,[0,\infty))(\psi_1^{-1})'(\lambda)|^{\eta_1}}{|\psi_1^{-1}(\lambda)|^{\eta_4}} |\psi_1^{-1}(\lambda)+1|^{\eta_2} |\psi_1^{-1}(\lambda)-1|^{\eta_3} \leq C|a|^{p-\alpha+\beta} K, \tag{4.4.9}$$

where $C = C(\alpha, \beta, p, \varepsilon, \tau)$. Recall that $\psi_1^{-1}(\lambda) = \frac{\sqrt{-\lambda}-b}{\sqrt{-\lambda}+b}$ where $b = \sqrt{-a}$. Since

$$(\psi_1^{-1})'(\lambda) = \frac{-b}{\sqrt{-\lambda}(\sqrt{-\lambda}+b)^2}$$

and

$$\psi_1^{-1}(\lambda) - 1 = \frac{-2b}{\sqrt{-\lambda}+b}, \quad \psi_1^{-1}(\lambda)+1 = \frac{2\sqrt{-\lambda}}{\sqrt{-\lambda}+b},$$

estimate (4.4.9) implies that

$$\sum_{\lambda \in \sigma_d(H)} \frac{\operatorname{dist}(\lambda,[0,\infty))^{\eta_1}}{|\lambda|^{\frac{\eta_1-\eta_2}{2}} |\sqrt{-\lambda}+b|^{2\eta_1+\eta_2+\eta_3-\eta_4} |\sqrt{-\lambda}-b|^{\eta_4}} \leq C|a|^{p-\alpha+\beta-\frac{\eta_1+\eta_3}{2}} K.$$

We conclude the proof by noting that

$$|\sqrt{-\lambda}-b| = \frac{|\lambda-a|}{|\sqrt{-\lambda}+b|} \quad \text{and} \quad |\sqrt{-\lambda}+b| \leq (|\lambda|^{1/2}+b) \leq 2(|\lambda|+|a|)^{1/2}. \quad \square$$

Remark 4.4.5. Analogous to our discussion in Remark 4.2.4, let us consider the consequences of estimate (4.4.7) for the discrete spectrum of H in a little more detail. To this end, let $\{\lambda_k\}$ be a sequence of isolated eigenvalues of H converging to some $\lambda^* \in [0,\infty)$. Taking a subsequence, we can suppose that one of the following options holds:

(i) $\lambda^* = 0$ and $\operatorname{Re}(\lambda_k) \leq 0$ (ii) $\lambda^* = 0$ and $\operatorname{Re}(\lambda_k) > 0$ (iii) $\lambda^* > 0$.

In case (i), since $\operatorname{dist}(\lambda_k,[0,\infty)) = |\lambda_k|$, (4.4.7) implies the finiteness of

$$\sum\nolimits_k |\lambda_k|^{(\eta_1+\eta_2)/2},$$

so any such sequence must converge to 0 sufficiently fast. Similarly, in case (ii), (4.4.7) implies the finiteness of $\sum_k |\operatorname{Im}(\lambda_k)|^{\eta_1} |\lambda_k|^{-(\eta_1-\eta_2)/2}$, and in case (iii) we obtain the finiteness of $\sum_k |\operatorname{Im}(\lambda_k)|^{\eta_1}$, which shows that any such sequence must converge to the real line sufficiently fast. Estimate (4.4.7) also provides information about divergent sequences of eigenvalues. For example, if $\{\lambda_k\}$ is an infinite sequence of eigenvalues which stays bounded away from $[0,\infty)$, that is, $\mathrm{dist}(\lambda_k,[0,\infty)) \geq \delta$ for some $\delta > 0$ and all k, then (4.4.7) implies that

$$\sum\nolimits_k \frac{1}{|\lambda_k|^{(3\eta_1+\eta_3)/2}} < \infty,$$

which shows that the sequence $\{\lambda_k\}$ must diverge to infinity sufficiently fast.

Estimate (4.4.7) provides us with a family of inequalities parameterized by $a < \omega$. By considering an average of all these inequalities, i.e., by multiplying both sides of (4.4.7) with an a-dependent weight and integrating with respect to a, it is possible to extract some more information on $\sigma_d(H)$. Of course, in this context, we have to be aware that the constants and parameters on the right-hand side of (4.4.7) may still depend on a. We can use the estimate (4.4.3) to get rid of this dependence.

Theorem 4.4.6. *Let $\omega \leq 0$ and $C_0 = C_0(\omega) > 0$ be chosen as in (4.4.2) and (4.4.3), respectively, and assume that for all $\lambda \in \mathbb{C} \setminus [0,\infty)$ we have*

$$\|MR_{H_0}(\lambda)\|^p_{\mathcal{S}_p} \leq \frac{K|\lambda|^\beta}{\mathrm{dist}(\lambda,[0,\infty))^\alpha}, \tag{4.4.10}$$

where $K \geq 0$, $\alpha > 0$ and $\beta \in \mathbb{R}$. Let $\tau > 0$ and define

$$\begin{aligned} \eta_0 &= -\alpha + \beta + \tau, \\ \eta_1 &= \alpha + 1 + \tau, \\ \eta_2 &= ((\alpha - 2\beta)_+ - 1 + \tau)_+. \end{aligned} \tag{4.4.11}$$

Then the following holds: If $\omega < 0$ then

$$\sum_{\lambda \in \sigma_d(H)} \frac{\mathrm{dist}(\lambda,[0,\infty))^{\eta_1}}{|\lambda|^{\frac{\eta_1-\eta_2}{2}}(|\lambda|+|\omega|)^{\eta_0+\frac{\eta_1+\eta_2}{2}}} \leq C\frac{C_0^p K}{|\omega|^\tau}. \tag{4.4.12}$$

If $\omega = 0$ then for $s > 0$

$$\sum_{\lambda \in \sigma_d(H), |\lambda|>s} \frac{\mathrm{dist}(\lambda,[0,\infty))^{\eta_1}}{|\lambda|^{\beta+1+2\tau}} + \sum_{\lambda \in \sigma_d(H), |\lambda| \leq s} \frac{\mathrm{dist}(\lambda,[0,\infty))^{\eta_1}}{|\lambda|^{\beta+1}s^{2\tau}} \leq C\frac{C_0^p K}{s^\tau}. \tag{4.4.13}$$

In both cases, $C = C(\alpha,\beta,p,\tau)$. Moreover, if $\alpha = 0$ then in (4.4.12) and (4.4.13) we can replace η_1 by 1.

Proof. By (4.4.3) we have, for $a < \omega$, $\|R_H(a)\| \leq C_0|a-\omega|^{-1}$, so (4.4.10) implies that

$$\|R_H(a)MR_{H_0}(\lambda)\|^p_{\mathcal{S}_p} \leq \frac{C_0^p K}{|a-\omega|^p}\frac{|\lambda|^\beta}{\mathrm{dist}(\lambda,[0,\infty))^\alpha}. \tag{4.4.14}$$

For $\varepsilon, \tau > 0$, let η_j, where $j = 1,\dots,4$, be defined by (4.4.6). Then Theorem 4.4.3 implies that

$$\sum_{\lambda \in \sigma_d(H)} \frac{\mathrm{dist}(\lambda,[0,\infty))^{\eta_1}}{|\lambda|^{\frac{\eta_1-\eta_2}{2}}(|\lambda|+|a|)^{\eta_1-\eta_4+\frac{\eta_2+\eta_3}{2}}|\lambda-a|^{\eta_4}} \leq \frac{C_0^p C(\alpha,\beta,p,\varepsilon,\tau)K}{|a|^{\frac{\eta_1+\eta_3}{2}-p+\alpha-\beta}|a-\omega|^p}.$$

Setting $\varepsilon = \tau$ and using that $|\lambda - a| \leq (|\lambda| + |a|)$ the last inequality implies that

$$\sum_{\lambda \in \sigma_d(H)} \frac{\operatorname{dist}(\lambda, [0,\infty))^{\eta_1}}{|\lambda|^{\frac{\eta_1-\eta_2}{2}} (|\lambda| + |a|)^{\eta_1 + \frac{\eta_2+\eta_3}{2}}} \leq \frac{C_0^p C(\alpha, \beta, p, \tau) K}{|a|^{\frac{\eta_1+\eta_3}{2} - p + \alpha - \beta} |a - \omega|^p}. \tag{4.4.15}$$

To simplify notation, we set $r = |a| (> |\omega|)$, $C = C(\alpha, \beta, p, \tau)$,

$$\varphi_1 = \frac{\eta_1 + \eta_3}{2} - p + \alpha - \beta \qquad \text{and} \qquad \varphi_2 = \eta_1 + \frac{\eta_2 + \eta_3}{2}.$$

Note that $\varphi_1, \varphi_2 > 0$. Now let us introduce some constant $s = s(\omega)$. More precisely, we choose $s = 0$ if $|\omega| > 0$ and $s > 0$ if $\omega = 0$. Then we can rewrite (4.4.15) as follows

$$\sum_{\lambda \in \sigma_d(H)} \frac{\operatorname{dist}(\lambda, [0,\infty))^{\eta_1} r^{\varphi_1 - 1 + \tau} (r - |\omega|)^p}{|\lambda|^{\frac{\eta_1-\eta_2}{2}} (|\lambda| + r)^{\varphi_2} (s + r)^{2\tau}} \leq \frac{C_0^p C K}{r^{1-\tau} (s + r)^{2\tau}}. \tag{4.4.16}$$

Next, we integrate both sides of the last inequality with respect to $r \in (|\omega|, \infty)$. We obtain for the right-hand side

$$\int_{|\omega|}^{\infty} \frac{dr}{r^{1-\tau}(s+r)^{2\tau}} = \begin{cases} \frac{1}{\tau |\omega|^\tau}, & |\omega| > 0 \text{ and } s = 0 \\ \frac{C(\tau)}{s^\tau}, & \omega = 0 \text{ and } s > 0. \end{cases} \tag{4.4.17}$$

Integrating the left-hand side of (4.4.16), interchanging sum and integral, it follows that

$$\begin{aligned} &\int_{|\omega|}^{\infty} dr \left(\sum_{\lambda \in \sigma_d(H)} \frac{\operatorname{dist}(\lambda, [0,\infty))^{\eta_1} r^{\varphi_1 - 1 + \tau} (r - |\omega|)^p}{|\lambda|^{\frac{\eta_1-\eta_2}{2}} (|\lambda| + r)^{\varphi_2} (s + r)^{2\tau}} \right) \\ &\quad = \sum_{\lambda \in \sigma_d(H)} \frac{\operatorname{dist}(\lambda, [0,\infty))^{\eta_1}}{|\lambda|^{\frac{\eta_1-\eta_2}{2}}} \int_{|\omega|}^{\infty} dr \frac{(r - |\omega|)^p r^{\varphi_1 - 1 + \tau}}{(|\lambda| + r)^{\varphi_2} (s + r)^{2\tau}}. \end{aligned} \tag{4.4.18}$$

We note that the finiteness of (4.4.18) is a consequence of (4.4.17) and (4.4.16). Substituting $t = \frac{r - |\omega|}{|\lambda| + |\omega|}$, we obtain for the integral in (4.4.18):

$$\begin{aligned} &\int_{|\omega|}^{\infty} dr \frac{(r - |\omega|)^p r^{\varphi_1 - 1 + \tau}}{(|\lambda| + r)^{\varphi_2} (s + r)^{2\tau}} \\ &\quad = \frac{1}{(|\lambda| + |\omega|)^{\varphi_2 - 1 - p}} \int_0^{\infty} dt \frac{t^p [(|\lambda| + |\omega|)t + |\omega|]^{\varphi_1 - 1 + \tau}}{(t+1)^{\varphi_2} [(|\lambda| + |\omega|)t + |\omega| + s]^{2\tau}} \\ &\quad \geq \frac{1}{(|\lambda| + |\omega|)^{\varphi_2 - \varphi_1 - p - \tau}} \int_0^{\infty} dt \frac{t^{p + \varphi_1 - 1 + \tau}}{(t+1)^{\varphi_2} [(|\lambda| + |\omega|)t + |\omega| + s]^{2\tau}} \\ &\quad \geq \frac{C(\alpha, \beta, p, \tau)}{(|\lambda| + |\omega|)^{\varphi_2 - \varphi_1 - p - \tau} \max(|\lambda| + |\omega|, s + |\omega|)^{2\tau}}. \end{aligned} \tag{4.4.19}$$

It remains to put together the information contained in (4.4.16)–(4.4.19) and to evaluate the constants (for instance, $\varphi_2 - \varphi_1 - p - \tau = \frac{\eta_1 + \eta_2}{2} + \eta_0 - 2\tau$). □

5. Eigenvalue estimates – an operator theoretic approach

In this chapter we will present our second approach for studying the distribution of eigenvalues of non-selfadjoint operators, based on material from [26]. As compared to the complex analysis method this approach is quite elementary but, as we will see, still strong enough to improve upon some features of the former method.

5.1. Kato's theorem

The estimate we are going to present in Section 5.2 will be a variant of the following classical estimate of Kato.

Theorem 5.1.1 ([32]). *Let $Z, Z_0 \in \mathcal{B}(\mathcal{H})$ be selfadjoint and assume that $Z - Z_0 \in \mathcal{S}_p(\mathcal{H})$ for some $p \geq 1$. Then there exist extended enumerations $\{z_j\}$ and $\{z_j^0\}$ of the discrete spectra of Z and Z_0, respectively, such that*

$$\sum_j |z_j - z_j^0|^p \leq \|Z - Z_0\|_{\mathcal{S}_p}^p. \tag{5.1.1}$$

Here an extended enumeration of the discrete spectrum is a sequence which contains all discrete eigenvalues, counting multiplicity, and which in addition might contain boundary points of the essential spectrum. An immediate consequence of Kato's theorem is

Corollary 5.1.2. *Let $Z, Z_0 \in \mathcal{B}(\mathcal{H})$ be selfadjoint and assume that $Z - Z_0 \in \mathcal{S}_p(\mathcal{H})$ for some $p \geq 1$. Then*

$$\sum_{\lambda \in \sigma_d(Z)} \operatorname{dist}(\lambda, \sigma(Z_0))^p \leq \|Z - Z_0\|_{\mathcal{S}_p}^p. \tag{5.1.2}$$

As it stands, Kato's theorem (and its corollary) need not be correct if (at least) one of the operators is non-selfadjoint. Indeed, even in the finite-dimensional case it can fail drastically.

Example 5.1.3. Let $\mathcal{H} = \mathbb{C}^2$ and for $a > 0$ define

$$Z_0 = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad Z = \begin{pmatrix} 0 & 1 \\ a & 0 \end{pmatrix}.$$

Then $\sigma_d(Z_0) = \{0\}$, $\sigma_d(Z) = \{\sqrt{a}, -\sqrt{a}\}$, $\|Z - Z_0\|_{\mathcal{S}_p}^p = a^p$ and

$$\sum_{\lambda \in \sigma_d(Z)} \operatorname{dist}(\lambda, \sigma_d(Z_0))^p = 2a^{p/2}.$$

Here for small a the quotient of left- and right-hand side in (5.1.2) can become arbitrarily large.

On the other hand, Kato's theorem is known to remain correct if Z_0, Z and $Z - Z_0$ are normal [2] or if Z_0, Z and $Z - Z_0$ are unitary [4], provided a multiplicative constant $\pi/2$ is added to the right-hand side. Inequality (5.1.2) remains valid if Z_0

and Z (but not necessarily $Z - Z_0$) are normal, but only if $p \geq 2$ [6]. Moreover, the slightly weaker estimate

$$\sum_{\lambda \in \sigma_d(Z)} \operatorname{dist}(\lambda, \sigma(Z_0))^p \leq C_p \|Z - Z_0\|_{\mathcal{S}_p}^p, \tag{5.1.3}$$

where the constant C_p is independent of Z_0 and Z, holds provided that Z_0 is selfadjoint and Z is normal [3].

The case of most interest to us is the case where Z_0 is selfadjoint (and its spectrum is an interval) and Z is arbitrary. In the next section we will show that in this case inequality (5.1.2) does indeed remain correct. As we will see, this will be a simple corollary of a much more general estimate.

Remark 5.1.4. Recently it has been shown [27] that for $p > 1$ estimate (5.1.3) remains valid if Z_0 is selfadjoint and Z is arbitrary, even without the additional assumption that $\sigma(Z_0)$ is an interval. We will come back to this result in Chapter 8.

5.2. An eigenvalue estimate involving the numerical range

The following theorem provides an estimate on the eigenvalues of Z given the mere assumption that $Z - Z_0$ is in $\mathcal{S}_p(\mathcal{H})$. In particular, it does *not* require that Z_0 is selfadjoint, normal or something alike.

Theorem 5.2.1 ([26]). *Let $Z_0, Z \in \mathcal{B}(\mathcal{H})$ and assume that $Z - Z_0 \in \mathcal{S}_p(\mathcal{H})$ for some $p \geq 1$. Then*

$$\sum_{\lambda \in \sigma_d(Z)} \operatorname{dist}(\lambda, \operatorname{Num}(Z_0))^p \leq \|Z - Z_0\|_{\mathcal{S}_p}^p. \tag{5.2.1}$$

The proof of this theorem will be given below.

Remark 5.2.2. It is interesting to observe that estimate (5.2.1) remains valid for $p \in (0, 1)$ if Z_0 and Z are selfadjoint. This is in contrast to Kato's theorem, which will not be correct in this case. We refer to [26] for a proof of these statements.

Since the closure of the numerical range of a normal operator coincides with the convex hull of its spectrum, the following corollary is immediate.

Corollary 5.2.3. *Let $Z_0, Z \in \mathcal{B}(\mathcal{H})$ and assume that $Z - Z_0 \in \mathcal{S}_p(\mathcal{H})$ for some $p \geq 1$. Moreover, let Z_0 be normal and assume that $\sigma(Z_0)$ is convex. Then*

$$\sum_{\lambda \in \sigma_d(Z)} \operatorname{dist}(\lambda, \sigma(Z_0))^p \leq \|Z - Z_0\|_{\mathcal{S}_p}^p. \tag{5.2.2}$$

In particular, as mentioned above, this corollary applies if Z_0 is selfadjoint and the spectrum of Z_0 is an interval.

Example 5.2.4. Let us take a second look at Example 4.1.6, where $Z_0 \in \mathcal{B}(\mathcal{H})$ was normal with $\sigma(Z_0) = \sigma_{\text{ess}}(Z_0) = \overline{\mathbb{D}}$ and $Z = Z_0 + M$ with $M \in \mathcal{S}_p(\mathcal{H})$ for some $p \geq 1$ (in particular, $\sigma_d(Z) \subset \overline{\mathbb{D}}^c$). The previous corollary then implies that

$$\sum_{\lambda \in \sigma_d(Z)} (|\lambda| - 1)^p \leq \|M\|_{\mathcal{S}_p}^p,$$

which is stronger than the corresponding estimate obtained in Example 4.1.6 via the complex analysis approach.

Remark 5.2.5. A version of Corollary 5.2.3 for unbounded operators will be provided in Section 5.3.

The proof of Theorem 5.2.1 relies on the following characterization of Schatten-p-norms, see [44] Proposition 2.6.

Lemma 5.2.6. *Let $K \in \mathcal{S}_p(\mathcal{H})$, where $p \geq 1$. Then*

$$\|K\|_{\mathcal{S}_p}^p = \sup_{\{e_i\},\{f_i\}} \left\{ \sum_i |\langle Ke_i, f_i \rangle|^p \right\},$$

where the supremum is taken with respect to arbitrary orthonormal sequences $\{e_i\}$ and $\{f_i\}$ in $\mathcal{H}$.

Proof of Theorem 5.2.1. Let $\Lambda = \{\lambda_1, \ldots, \lambda_n\}$ be an arbitrary finite subset of $\sigma_d(Z)$ and let

$$P_Z(\Lambda) = P_Z(\lambda_1) + \ldots + P_Z(\lambda_n)$$

be the corresponding Riesz-Projection. Then $N := \text{Rank}(P_Z(\Lambda))$ is the sum of the (algebraic) multiplicities of the λ_i's and, invoking Schur's lemma, we can find an orthonormal basis $\{e_1, \ldots, e_N\}$ of $\text{Ran}(P_Z(\Lambda))$ such that

$$Ze_i = z_{i1}e_1 + z_{i2}e_2 + \ldots + z_{ii}e_i \qquad i = 1, \ldots, N, \tag{5.2.3}$$

where the z_{ii}'s are the eigenvalues in Λ, counted according to their multiplicity (in other words, the finite-dimensional operator $Z|_{\text{Ran}(P_Z(\Lambda))}$ has upper-triangular form). Applying Lemma 5.2.6 to this particular sequence $\{e_i\}$ we obtain

$$\|Z - Z_0\|_{\mathcal{S}_p}^p \geq \sum_{i=1}^N |\langle (Z - Z_0)e_i, e_i \rangle|^p = \sum_{i=1}^N |\langle Ze_i, e_i \rangle - \langle Z_0 e_i, e_i \rangle|^p.$$

But $\langle Ze_i, e_i \rangle = z_{ii}$ and $\langle Z_0 e_i, e_i \rangle \in \text{Num}(Z_0)$, so the previous estimate implies that

$$\sum_{\lambda \in \Lambda} \text{dist}(\lambda, \text{Num}(Z_0))^p \leq \|Z - Z_0\|_{\mathcal{S}_p}^p,$$

where each eigenvalue is counted according to its multiplicity. Noting that the right-hand side is independent of Λ concludes the proof of Theorem 5.2.1. □

Remark 5.2.7. The method of proof of Theorem 5.2.1 can also be used to recover another recent result about the distribution of eigenvalues of non-selfadjoint operators, by Bruneau and Ouhabaz [7, Theorem 1]. Let H be an m-sectorial operator in $\mathcal{H}$ with the associated sesquilinear form $h(u, v)$ and let $\text{Re}(H)$ denote the real part of H, i.e., the selfadjoint operator associated to the form $1/2(h(u, v) + \overline{h(v, u)})$.

For simplicity, let us suppose that $\mathrm{Dom}(H) \subset \mathrm{Dom}(\mathrm{Re}(H))$. Then, assuming that the negative part $\mathrm{Re}(H)_-$ of $\mathrm{Re}(H)$ is in $\mathcal{S}_p(\mathcal{H})$, we obtain as above that

$$\sum_{i=1}^{N} |\langle \mathrm{Re}(H)e_i, e_i\rangle - \langle \mathrm{Re}(H)_+ e_i, e_i\rangle|^p \leq \|\mathrm{Re}(H)_-\|_{\mathcal{S}_p}^p,$$

where $\{e_i\}$ is a Schur basis corresponding to a finite number of eigenvalues $(\lambda_i)_{i=1}^N$ of H with $\mathrm{Re}(\lambda_i) < 0$. Since $\langle \mathrm{Re}(H)e_i, e_i\rangle = \mathrm{Re}(\lambda_i)$ and $\langle \mathrm{Re}(H)_+ e_i, e_i\rangle \geq 0$ this estimate implies that $\sum_{i=1}^N |\mathrm{Re}(\lambda_i)|^p \leq \|\mathrm{Re}(H)_-\|_{\mathcal{S}_p}^p$ and so we arrive at the estimate

$$\sum_{\lambda \in \sigma_d(H), \mathrm{Re}(\lambda)<0} |\mathrm{Re}(\lambda)|^p \leq \|\mathrm{Re}(H)_-\|_{\mathcal{S}_p}^p, \tag{5.2.4}$$

the result of Bruneau and Ouhabaz.

5.3. Perturbations of non-negative operators

With the help of resolvents we can transfer the eigenvalue estimates of the previous section to unbounded operators. To make things simple, we will only study perturbations of non-negative operators.

Theorem 5.3.1. *Let $H_0 \in \mathcal{C}(\mathcal{H})$ be selfadjoint with $\sigma(H_0) \subset [0, \infty)$. Let $H \in \mathcal{C}(\mathcal{H})$ and assume that $a \in \rho(H) \cap (-\infty, 0)$. If $R_H(a) - R_{H_0}(a) \in \mathcal{S}_p(\mathcal{H})$ for some $p \geq 1$, then*

$$\sum_{\lambda \in \sigma_d(H)} \frac{\mathrm{dist}(\lambda, [0,\infty))^p}{|\lambda + a|^p (|\lambda| + |a|)^p} \leq 8^p \|R_H(a) - R_{H_0}(a)\|_{\mathcal{S}_p}^p. \tag{5.3.1}$$

Remark 5.3.2. If we restrict the sum on the left-hand side of (5.3.1) to eigenvalues in the right half-plane, then the estimate remains valid without the additional constant 8^p on the right-hand side, see [26, Theorem 3.1].

Proof. Applying Corollary 5.2.3 to $Z = R_H(a)$ and $Z_0 = R_{H_0}(a)$ we obtain

$$\sum_{\mu \in \sigma_d(R_H(a))} \mathrm{dist}(\mu, \sigma(R_{H_0}(a)))^p \leq \|R_H(a) - R_{H_0}(a)\|_{\mathcal{S}_p}^p.$$

The spectral mapping theorem and the assumption $\sigma(H_0) \subset [0, \infty)$ imply that $\sigma(R_{H_0}(a)) \subset [a^{-1}, 0]$, so applying the spectral mapping theorem again we obtain

$$\sum_{\lambda \in \sigma_d(H)} \mathrm{dist}((a-\lambda)^{-1}, [a^{-1}, 0])^p \leq \|R_H(a) - R_{H_0}(a)\|_{\mathcal{S}_p}^p.$$

All that remains is to observe that

$$\mathrm{dist}\left((a-\lambda)^{-1}, [a^{-1}, 0]\right) \geq \frac{1}{8} \frac{\mathrm{dist}(\lambda, [0,\infty))}{|\lambda + a|(|\lambda| + |a|)},$$

see the proof of Theorem 3.3.1 in [25]. □

In applications to, for instance, Schrödinger operators, estimates on the Schatten norm on the right-hand side of (5.3.1) will take a particular form, namely, we will have that

$$\|R_H(a) - R_{H_0}(a)\|_{\mathcal{S}_p}^p \leq C_0 |a|^{-\alpha}(|a| - |\omega|)^{-\beta}$$

for some constants $\alpha, \beta \geq 0$, $C_0 > 0$, $\omega < 0$ and every $a \in (-\infty, \omega)$ (compare this with (4.4.5) and (4.4.10)). Note that α, β and C_0 may depend on p but *not* on a. In particular, in this case Theorem 5.3.1 provides us with a whole family of estimates (i.e., one estimate for every $a < -\omega$) and we can take advantage of this fact by taking a suitable average of all these estimates, similar to what we have done in the derivation of Theorem 4.4.6. This is the content of the next theorem.

Theorem 5.3.3. *Let $H_0 \in \mathcal{C}(\mathcal{H})$ be selfadjoint with $\sigma(H_0) \subset [0, \infty)$ and let $H \in \mathcal{C}(\mathcal{H})$ with $(-\infty, \omega) \subset \rho(H)$ for some $\omega \leq 0$. Suppose that for some $p \geq 1$ there exist $\alpha, \beta \geq 0$ and $C_0 > 0$ such that for every $a < \omega$ we have*

$$\|R_H(a) - R_{H_0}(a)\|_{\mathcal{S}_p}^p \leq C_0 |a|^{-\alpha}(|a| - |\omega|)^{-\beta}. \tag{5.3.2}$$

Then for every $\tau > 0$ the following holds: If $\omega < 0$ then

$$\sum_{\lambda \in \sigma_d(H)} \frac{\operatorname{dist}(\lambda, [0, \infty))^p}{(|\lambda| + |\omega|)^{-\alpha - \beta + 2p + \tau}} \leq C_0 C(\alpha, \beta, \tau, p) |\omega|^{-\tau}. \tag{5.3.3}$$

If $\omega = 0$ then for $s > 0$

$$\sum_{\substack{\lambda \in \sigma_d(H) \\ |\lambda| > s}} \frac{\operatorname{dist}(\lambda, [0, \infty))^p}{|\lambda|^{-\alpha - \beta + 2p + \tau}} + \sum_{\substack{\lambda \in \sigma_d(H) \\ |\lambda| \leq s}} \frac{\operatorname{dist}(\lambda, [0, \infty))^p}{|\lambda|^{-\alpha - \beta + 2p - \tau} s^{2\tau}} \leq C_0 s^{-\tau} C(\alpha, \beta, \tau, p). \tag{5.3.4}$$

Proof. From Theorem 5.3.1 and our assumption we obtain

$$\sum_{\lambda \in \sigma_d(H)} \frac{\operatorname{dist}(\lambda, [0, \infty))^p}{|\lambda + a|^p (|\lambda| + |a|)^p} \leq 8^p C_0 |a|^{-\alpha}(|a| - |\omega|)^{-\beta},$$

which we can rewrite as (also using the triangle inequality $|a + \lambda| \leq |a| + |\lambda|$)

$$\sum_{\lambda \in \sigma_d(H)} \frac{\operatorname{dist}(\lambda, [0, \infty))^p |a|^{\alpha - 1 + \tau}(|a| - |\omega|)^\beta}{(|\lambda| + |a|)^{2p}(s + |a|)^{2\tau}} \leq 8^p C_0 |a|^{-1+\tau}(s + |a|)^{-2\tau},$$

where we choose $s = 0$ if $|\omega| > 0$ and $s > 0$ if $\omega = 0$. Integrating with respect to $r := |a|$ we obtain

$$\sum_{\lambda \in \sigma_d(H)} \operatorname{dist}(\lambda, [0, \infty))^p \int_{|\omega|}^\infty dr \frac{r^{\alpha - 1 + \tau}(r - |\omega|)^\beta}{(|\lambda| + r)^{2p}(s + r)^{2\tau}} \leq C_0 8^p \int_{|\omega|}^\infty dr \frac{1}{r^{1-\tau}(s + r)^{2\tau}}.$$

As in the proof of Theorem 4.4.6 we can estimate the integral on the left from below by

$$\frac{C(\alpha, \beta, p, \tau)}{(|\lambda| + |\omega|)^{-\alpha - \beta + 2p - \tau} \max(|\lambda| + |\omega|, s + |\omega|)^{2\tau}},$$

and the integral on the right is equal to

$$\begin{cases} \frac{1}{\tau|\omega|^\tau}, & |\omega|>0 \text{ and } s=0 \\ \frac{C(\tau)}{s^\tau}, & \omega=0 \text{ and } s>0. \end{cases}$$

Putting everything together concludes the proof. □

6. Comparing the two approaches

Above we have developed two quite different approaches for obtaining inequalities involving the eigenvalues of non-selfadjoint operators. One is based on applying complex-analysis theorems on the distribution of zeros of holomorphic functions to perturbation determinants (Chapter 4), and the other relies on direct operator-theoretic arguments involving the numerical range (Chapter 5). We now wish to compare the results obtained by the two methods, in order to understand the strengths and limitations of each approach.

We consider only the case in which A_0 is a bounded self-adjoint operator, with $\sigma(A_0)=[a,b]$, and $A=A_0+M$, where $M\in\mathcal{S}_p(\mathcal{H})$. Corollary 4.2.5, obtained using the complex-analysis approach, tells us that, when $p\geq 1$ and for any $\tau>0$ we have

$$\sum_{\lambda\in\sigma_d(A)} \frac{\operatorname{dist}(\lambda,[a,b])^{p+1+\tau}}{|\lambda-b||\lambda-a|} \leq C(p,\tau)(b-a)^{-1+\tau}\|M\|_{\mathcal{S}_p}^p \tag{6.1}$$

and that when $p<1$, and $0<\tau<1-p$,

$$\sum_{\lambda\in\sigma_d(A)} \left(\frac{\operatorname{dist}(\lambda,[a,b])}{|b-\lambda|^{1/2}|a-\lambda|^{1/2}}\right)^{p+1+\tau} \leq C(p,\tau)(b-a)^{-p}\|M\|_{\mathcal{S}_p}^p. \tag{6.2}$$

Corollary 5.2.3, obtained using the numerical range approach, tells us that

$$\sum_{\lambda\in\sigma_d(A)} \operatorname{dist}(\lambda,[a,b])^p \leq \|M\|_{\mathcal{S}_p}^p. \tag{6.3}$$

Clearly a good feature of (6.3), as opposed to (6.1), is the absence of a constant C on the right-hand side. An optimal value of the constant $C(p,\tau)$ in (6.1) is not known, and though explicit upper bounds for such an optimal value could be extracted by making all the estimates used in its derivation explicit, the resulting expression would be complicated, and there is little reason to expect that it would yield a sharp result.

We now compare the information that can be deduced from these inequalities regarding the asymptotic behavior of sequences of eigenvalues.

(i) Assume first that $p\geq 1$. To begin with consider a sequence of eigenvalues $\{\lambda_k\}$ with $\lambda_k\to\lambda^*\in(a,b)$ as $k\to\infty$. Then $|\lambda_k-a|$ and $|\lambda_k-b|$ are bounded from below by some positive constant, hence we conclude from (6.1) that the sum $\sum_{k=1}^\infty \operatorname{dist}(\lambda_k,[a,b])^{p+1+\tau}$ is finite, for any $\tau>0$. However, (6.3) implies the finiteness of $\sum_{k=1}^\infty \operatorname{dist}(\lambda_k,[a,b])^p$, obviously a stronger result.

If we consider a sequence $\{\lambda_k\}$ with $\lambda_k \to a$, then (6.1) implies

$$\sum_{k=1}^{\infty} \frac{\text{dist}(\lambda_k, [a,b])^{p+1+\tau}}{|a-\lambda_k|} < \infty,$$

for any $\tau > 0$. However, since $|\lambda_k - a| \geq \text{dist}(\lambda_k, [a,b])$, so that

$$\text{dist}(\lambda_k, [a,b])^p \geq \frac{\text{dist}(\lambda_k, [a,b])^{p+1}}{|\lambda_k - a|}$$

(6.3) implies the stronger result

$$\sum_{k=1}^{\infty} \frac{\text{dist}(\lambda_k, [a,b])^{p+1}}{|\lambda_k - a|} < \infty.$$

Thus, we have established the superiority of (6.3) over (6.1).

(ii) Let us examine the case $0 < p < 1$, $0 < \tau < 1 - p$. Corollary 5.2.3 is not valid for $p < 1$, but we can use the fact that $\mathcal{S}_p(\mathcal{H}) \subset \mathcal{S}_1(\mathcal{H})$ to conclude that

$$\sum_{\lambda \in \sigma_d(A)} \text{dist}(\lambda, [a,b]) \leq \|M\|_{\mathcal{S}_1}. \tag{6.4}$$

Considering a sequence $\{\lambda_k\}$ of eigenvalues with $\lambda_k \to \lambda^* \in (a,b)$ as $k \to \infty$, (6.2) implies $\sum_{k=1}^{\infty} \text{dist}(\lambda_k, [a,b])^{p+1+\tau} < \infty$, which is weaker than the result

$$\sum_{k=1}^{\infty} \text{dist}(\lambda_k, [a,b]) < \infty$$

implied by (6.4).

However, considering a sequence $\{\lambda_k\}$ of eigenvalues with $\lambda_k \to a$ as $k \to \infty$, (6.2) gives

$$\sum_{k=1}^{\infty} \left(\frac{\text{dist}(\lambda_k, [a,b])}{|\lambda_k - a|^{\frac{1}{2}}} \right)^{p+1+\tau} < \infty. \tag{6.5}$$

This result does *not* follow from (6.4). To see this, take a real sequence with $\lambda_k < a$, so that $|\lambda_k - a| = \text{dist}(\lambda_k, [a,b])$. Then (6.5) becomes

$$\sum_{k=1}^{\infty} \text{dist}(\lambda_k, [a,b])^{\frac{1}{2}(p+1+\tau)} < \infty,$$

which is stronger than the result given by (6.4) since $p + \tau < 1$ implies that $\frac{1}{2}(p+1+\tau) < 1$.

Summing up, we have seen that in nearly all cases Corollary 5.2.3, proved by the numerical range approach, provides sharper information on the asymptotics of eigenvalue sequences than provided by Corollary 4.2.5, proved by the complex analysis approach, the sole exception being the case $p < 1$ when considering a sequence of eigenvalues converging to an edge of the essential spectrum.

This, however, is not the end of the story. Corollary 4.2.5 which we have been discussing, is only the simplest result that we can obtain using the complex analysis approach. We recall that Theorem 4.2.2, which provides inequalities on the eigenvalues assuming an estimate on the quantity $\|M_2 R_{A_0}(\lambda) M_1\|_{\mathcal{S}_p}^p$, where M_1, M_2 are a pair of operators with $M_1 M_2 = M$. Corollary 4.2.5 was obtained by taking $M_1 = I, M_2 = M$. As we shall see in Chapter 7.1, in an application to Jacobi operators, by choosing a different decomposition $M = M_1 M_2$ one may use Theorem 4.2.2 to obtain stronger results than those provided by Corollaries 4.2.5 and 5.2.3.

We may thus conclude that if one is considering a general bounded operator of the form $A = A_0 + M$, with A_0 selfadjoint, $\sigma(A_0) = [a, b]$, and $M \in \mathcal{S}_p(\mathcal{H})$, $p \geq 1$, and the only quantitative information available is a bound on the norm $\|M\|_{\mathcal{S}_p}$, then the best estimate on the discrete spectrum of A is provided by the numerical range method. If, however, one is dealing with specific classes of operators of the above form which have a special structure which allows to perform an appropriate decomposition $M = M_1 M_2$ and estimate $\|M_2 R_{A_0}(\lambda) M_1\|_{\mathcal{S}_p}^p$, one can sometimes obtain stronger results using the complex analysis approach (Theorem 4.2.2).

Remark. What has been said in the last paragraph applies also to the case of unbounded operators, as we will see in our discussion of Schrödinger operators in Chapter 7.2.

7. Applications

In this chapter we will finally apply our abstract estimates to some more concrete situations. Namely, we will analyze the discrete eigenvalues of bounded Jacobi operators on $l^2(\mathbb{Z})$ and of unbounded Schrödinger operators in $L^2(\mathbb{R}^d)$, respectively.

7.1. Jacobi operators

In this section, which is based on [28], we apply our general results on bounded non-selfadjoint perturbations of selfadjoint operators to obtain estimates on the discrete spectrum of complex Jacobi operators.

The spectral theory of Jacobi operators is a classical subject with many beautiful results, though by far the majority of results relate to selfadjoint Jacobi operators. Using our results, we are able to obtain new estimates on the eigenvalues of non-selfadjoint Jacobi operators which are nearly as strong as those which have been obtained in the selfadjoint case. The techniques, however, are very different, as previous results for the selfadjoint case have been obtained by methods which rely very strongly on the selfadjointness. This example thus gives a striking illustration of the utility of our general results in studying a concrete class of operators.

Another interesting feature of these results is that they provide an example in which the results proved by means of the complex-analysis approach of Chapter 4 are (in many respects) stronger than those we can obtain at present using the operator-theoretic approach of Chapter 5. This is in contrast with the case of 'general' operators, for which, as we have discussed above, the operator-theory approach provides results which are usually stronger.

Given three bounded complex sequences $\{a_k\}_{k\in\mathbb{Z}}$, $\{b_k\}_{k\in\mathbb{Z}}$ and $\{c_k\}_{k\in\mathbb{Z}}$, we define the associated (complex) *Jacobi operator* $J = J(a_k, b_k, c_k) : l^2(\mathbb{Z}) \to l^2(\mathbb{Z})$ as follows:

$$(Ju)(k) = a_{k-1}u(k-1) + b_k u(k) + c_k u(k+1), \quad u \in l^2(\mathbb{Z}). \tag{7.1.1}$$

It is easy to see that J is a bounded operator on $l^2(\mathbb{Z})$ with

$$\|J\| \leq \sup_k |a_k| + \sup_k |b_k| + \sup_k |c_k|.$$

Moreover, with respect to the standard basis $\{\delta_k\}_{k\in\mathbb{Z}}$ of $l^2(\mathbb{Z})$, i.e., $\delta_k(j) = 0$ if $j \neq k$ and $\delta_k(k) = 1$, J can be represented by the two-sided infinite tridiagonal matrix

$$\begin{pmatrix} \ddots & \ddots & \ddots & & & & \\ & a_{-1} & b_0 & c_0 & & & \\ & & a_0 & b_1 & c_1 & & \\ & & & a_1 & b_2 & c_2 & \\ & & & & \ddots & \ddots & \ddots \end{pmatrix}.$$

In view of this representation it is also customary to refer to J as a *Jacobi matrix.*

Example 7.1.1. The *discrete Laplace operator* on $l^2(\mathbb{Z})$ coincides with the Jacobi operator $J(1, -2, 1)$. Similarly, the Jacobi operator $J(-1, 2 + d_k, -1)$ ($d_k \in \mathbb{C}$) describes a *discrete Schrödinger operator.*

In the following, we will focus on Jacobi operators which are perturbations of the *free* Jacobi operator $J_0 = J(1, 0, 1)$, i.e.,

$$(J_0 u)(k) = u(k-1) + u(k+1), \quad u \in l^2(\mathbb{Z}). \tag{7.1.2}$$

More precisely, if $J = J(a_k, b_k, c_k)$ is defined as above, then throughout this section we assume that $J - J_0$ is compact.

Proposition 7.1.2. *The operator $J - J_0$ is compact if and only if*

$$\lim_{|k|\to\infty} a_k = \lim_{|k|\to\infty} c_k = 1 \quad \textit{and} \quad \lim_{|k|\to\infty} b_k = 0. \tag{7.1.3}$$

Proof. It is easy to see that $J - J_0$ is a norm limit of finite rank operators, and hence compact, if (7.1.3) is satisfied. On the other hand, if $J - J_0$ is compact then it maps weakly convergent zero-sequences into norm convergent zero-sequences. In particular,

$$\|(J - J_0)\delta_k\|_{l^2}^2 = |a_k - 1|^2 + |b_k|^2 + |c_{k-1} - 1|^2 \overset{|k|\to\infty}{\longrightarrow} 0$$

as desired. □

Let $F : l^2(\mathbb{Z}) \to L^2(0, 2\pi)$ denote the Fourier transform, i.e.,

$$(Fu)(\theta) = \frac{1}{\sqrt{2\pi}} \sum_{k\in\mathbb{Z}} e^{ik\theta} u_k.$$

Then for $u \in l^2(\mathbb{Z})$ and $\theta \in [0, 2\pi)$ we have

$$(FJ_0u)(\theta) = 2\cos(\theta)(Fu)(\theta), \tag{7.1.4}$$

as a short computation shows. In particular, we see that J_0 is unitarily equivalent to the operator of multiplication by the function $2\cos(\theta)$ on $L^2(0, 2\pi)$, and so the spectrum of J_0 coincides with the interval $[-2, 2]$. Consequently, the compactness of $J - J_0$ implies that

$$\sigma(J) = [-2, 2] \,\dot{\cup}\, \sigma_d(J),$$

i.e., the isolated eigenvalues of J are situated in $\mathbb{C} \setminus [-2, 2]$ and can accumulate on $[-2, 2]$ only.

Our aim is to derive estimates on $\sigma_d(J)$ given the stronger assumption that $J - J_0 \in \mathcal{S}_p$ (for simplicity, in this section we set $\mathcal{S}_p = \mathcal{S}_p(l^2(\mathbb{Z}))$. To this end, let us define a sequence $v = \{v_k\}_{k\in\mathbb{Z}}$ by setting

$$v_k = \max\Big(|a_{k-1} - 1|, |a_k - 1|, |b_k|, |c_{k-1} - 1|, |c_k - 1|\Big). \tag{7.1.5}$$

Clearly, the compactness of $J - J_0$ is equivalent to v_k converging to 0. Moreover, for $p \geq 1$ we will show in Lemma 7.1.3 below that $J - J_0 \in \mathcal{S}_p$ if and only if $v \in l^p(\mathbb{Z})$, and the $\mathcal{S}_p$-norm of $J - J_0$ and the l^p-norm of v are equivalent. If $p \in (0, 1)$, then the $\mathcal{S}_p$-norm of $J - J_0$ and the l^p-norm of v are still equivalent in the diagonal case when $a_k = c_k \equiv 1$. In general, however, we only obtain a one-sided estimate.

Lemma 7.1.3 ([28], Lemma 8). *Let $p > 0$. Then*

$$\|J - J_0\|_{\mathcal{S}_p} \leq 3\|v\|_{l^p}. \tag{7.1.6}$$

Moreover, if $p \geq 1$ then

$$6^{-1/p}\|v\|_{l^p} \leq \|J - J_0\|_{\mathcal{S}_p}. \tag{7.1.7}$$

From the above estimate and Corollary 4.2.5 we obtain

Theorem 7.1.4. *Let $\tau \in (0, 1)$. If $p \geq 1 - \tau$ then*

$$\sum_{\lambda\in\sigma_d(J)} \frac{\operatorname{dist}(\lambda, [-2, 2])^{p+1+\tau}}{|\lambda^2 - 4|} \leq C(\tau, p)\|v\|_{l_p}^p. \tag{7.1.8}$$

Moreover, if $p \in (0, 1 - \tau)$ then

$$\sum_{\lambda\in\sigma_d(J)} \left(\frac{\operatorname{dist}(\lambda, [-2, 2])}{|\lambda^2 - 4|^{1/2}}\right)^{p+1+\tau} \leq C(\tau, p)\|v\|_{l_p}^p. \tag{7.1.9}$$

Remark 7.1.5. A slightly weaker version of the previous theorem has first been obtained by Golinskii, Borichev and Kupin, compare Remark 4.2.7.

In addition, Corollary 5.2.3 implies

Theorem 7.1.6. *If $p \geq 1$ then*

$$\sum_{\lambda\in\sigma_d(J)} \operatorname{dist}(\lambda, [-2, 2])^p \leq \|v\|_{l_p}^p. \tag{7.1.10}$$

As was already discussed in Chapter 6, the result of Theorem 7.1.6 is stronger than that of Theorem 7.1.4 in the case $p \geq 1$. However, we now show that both of these results can be considerably improved, when $p \geq 1$, by a more refined application of Theorem 4.2.2. The following theorem is our main result on the discrete eigenvalues of Jacobi operators. Its proof will be presented below.

Theorem 7.1.7. *Let $\tau \in (0,1)$. If $v \in l^p(\mathbb{Z})$, where $p > 1$, then*

$$\sum_{\lambda \in \sigma_d(J)} \frac{\operatorname{dist}(\lambda, [-2,2])^{p+\tau}}{|\lambda^2 - 4|^{1/2}} \leq C(p,\tau)\|v\|_{l^p}^p. \tag{7.1.11}$$

Furthermore, if $v \in l^1(\mathbb{Z})$ then

$$\sum_{\lambda \in \sigma_d(J)} \frac{\operatorname{dist}(\lambda, [-2,2])^{1+\tau}}{|\lambda^2 - 4|^{\frac{1}{2}+\frac{\tau}{4}}} \leq C(\tau)\|v\|_{l^1}. \tag{7.1.12}$$

Let us compare the previous theorem with Theorem 7.1.4 and 7.1.6, respectively. To begin, we note that a direct calculation shows that for $\tau > 0$, $\lambda \in \mathbb{C} \setminus [-2,2]$ and $p > 1$ we have

$$\frac{\operatorname{dist}(\lambda, [-2,2])^{p+1+\tau}}{|\lambda^2 - 4|} \leq \frac{\operatorname{dist}(\lambda, [-2,2])^{p+\tau}}{|\lambda^2 - 4|^{1/2}}.$$

Moreover, if $\lambda \in \mathbb{C} \setminus [-2,2]$ and $|\lambda| \leq \|J\|$, then

$$\frac{\operatorname{dist}(\lambda, [-2,2])^{2+\tau}}{|\lambda^2 - 4|} \leq C(\tau, \|J\|) \frac{\operatorname{dist}(\lambda, [-2,2])^{1+\tau}}{|\lambda^2 - 4|^{\frac{1}{2}+\frac{\tau}{4}}}.$$

Hence, inequalities (7.1.11) and (7.1.12) provide more information on the discrete spectrum of J than inequality (7.1.8), i.e., Theorem 7.1.7 is stronger than Theorem 7.1.4.

The advantage of Theorem 7.1.7 over Theorem 7.1.6 can be seen by considering sequences of eigenvalues $\{\lambda_k\}$ converging to an endpoint of the spectrum. If $\lambda_k \to 2$ as $k \to \infty$, Theorem 7.1.6 implies the convergence of the sum $\sum_{k=1}^\infty |\lambda_k - 2|^p$, while Theorem 7.1.7 implies the convergence of the sum $\sum_{k=1}^\infty |\lambda_k - 2|^{p-\frac{1}{2}+\tau}$, which is strictly stronger when $\tau < \frac{1}{2}$.

It should be noted, however, that Theorem 7.1.7 does not subsume Theorem 7.1.6, since for sequences $\lambda_k \to (-2,2)$, Theorem 7.1.7 only implies the convergence of $\sum_{k=1}^\infty |\lambda_k - 2|^{p+\tau}$ for any $\tau > 0$, which is weaker than the convergence of $\sum_{k=1}^\infty |\lambda_k - 2|^p$ given by Theorem 7.1.6.

Problem 7.1.8. *In view of the previous discussion it is natural to conjecture that a result implying both Theorem* 7.1.6 *and* 7.1.7 *is true, namely the inequality obtained by setting $\tau = 0$ in* (7.1.11)*:*

$$\sum_{\lambda \in \sigma_d(J)} \frac{\operatorname{dist}(\lambda, [-2,2])^{p}}{|\lambda^2 - 4|^{1/2}} \leq C(p)\|v\|_{l^p}^p. \tag{7.1.13}$$

However, we have not been able to prove such a result, and it remains an open question. We note here that in the case of selfadjoint J, (7.1.13) *was proved by Hundertmark and Simon* [30]*. It was then partly extended to the non-selfadjoint case by Golinskii and Kupin* [22]*, who considered eigenvalues outside a diamond-shaped region avoiding the interval* $[-2,2]$*. We can therefore consider Theorem* 7.1.7 *as a near-generalization of the results of Hundertmark and Simon* (*and Golinskii and Kupin*)*, and it would be interesting to understand whether the gap between our result* (*with* $\tau > 0$) *and their results* ($\tau = 0$) *can be closed for general non-selfadjoint Jacobi operators.*

Proof of Theorem 7.1.7. Some of the technical results needed will be quoted without proofs, for which we will refer to [28].

Let the multiplication operator $M_v \in \mathcal{B}(l^2(\mathbb{Z}))$ be defined by $M_v\delta_k = v_k\delta_k$, where the sequence $v = \{v_k\}$ was defined in (7.1.5). Furthermore, we define the operator $U \in \mathcal{B}(l^2(\mathbb{Z}))$ by setting

$$U\delta_k = u_k^-\delta_{k-1} + u_k^0\delta_k + u_k^+\delta_{k+1},$$

where (using the convention that $\frac{0}{0} = 1$)

$$u_k^- = \frac{c_{k-1}-1}{\sqrt{v_{k-1}v_k}}, \quad u_k^0 = \frac{b_k}{v_k} \quad \text{and} \quad u_k^+ = \frac{a_k-1}{\sqrt{v_{k+1}v_k}}.$$

It is then easily checked that

$$J - J_0 = M_{v^{1/2}}UM_{v^{1/2}}, \tag{7.1.14}$$

where $v^{1/2} = \{v_k^{1/2}\}$. Moreover, the definition of $\{v_k\}$ implies that

$$|u_k^-| \le 1, \quad |u_k^0| \le 1 \quad \text{and} \quad |u_k^+| \le 1,$$

showing that $\|U\| \le 3$.

We intend to prove Theorem 7.1.7 by an application of Theorem 4.2.2. Since we have seen above that $J - J_0 = M_{v^{1/2}}UM_{v^{1/2}}$, we will apply that theorem choosing (with the notation of that theorem) $M_1 = M_{v^{1/2}}$ and $M_2 = UM_{v^{1/2}}$, and so we need an appropriate bound on the Schatten norm of $UM_{v^{1/2}}R_{J_0}(\lambda)M_{v^{1/2}}$.

Lemma 7.1.9. *Let $v \in l^p(\mathbb{Z})$, where $p \ge 1$. Then the following holds: if $p > 1$ then*

$$\|UM_{v^{1/2}}R_{J_0}(\lambda)M_{v^{1/2}}\|_{\mathcal{S}_p}^p \le \frac{C(p)\|v\|_{l^p}^p}{\operatorname{dist}(\lambda,[-2,2])^{p-1}|\lambda^2-4|^{1/2}}. \tag{7.1.15}$$

Furthermore, if $v \in l^1(\mathbb{Z})$, then for every $\varepsilon \in (0,1)$ we have

$$\|UM_{v^{1/2}}R_{J_0}(\lambda)M_{v^{1/2}}\|_{\mathcal{S}_1} \le \frac{C(\varepsilon)\|v\|_{l^1}}{\operatorname{dist}(\lambda,[-2,2])^{\varepsilon}|\lambda^2-4|^{(1-\varepsilon)/2}}. \tag{7.1.16}$$

The proof of Lemma 7.1.9 will be given below. First, let us continue with the proof of Theorem 7.1.7. To this end, let us assume that $v \in l^p(\mathbb{Z})$ and let us fix $\tau \in (0,1)$. Considering the case $p > 1$ first, we obtain from (7.1.15) and

Theorem 4.2.2, with $\alpha = p-1$, $\beta = -1/2$ and $K = C(p)\|v\|_{l^p}^p$, i.e., $\eta_1 = p+\tau$ and $\eta_2 = p-1+\tau$,

$$\sum_{\lambda \in \sigma_d(J)} \frac{\operatorname{dist}(\lambda, [-2,2])^{p+\tau}}{|\lambda^2-4|^{1/2}} \leq C(p,\tau)\|v\|_{l^p}^p.$$

Similarly, if $p = 1$, then we obtain from (7.1.16) and Theorem 4.2.2 that, for $\varepsilon \in (0,1)$ and $\tilde{\tau} \in (0,1)$,

$$\sum_{\lambda \in \sigma_d(J)} \frac{\operatorname{dist}(\lambda, [-2,2])^{1+\varepsilon+\tilde{\tau}}}{|\lambda^2-4|^{(1+\varepsilon)/2}} \leq C(\tilde{\tau},\varepsilon)\|v\|_{l^1}.$$

Choosing $\varepsilon = \tilde{\tau} = \tau/2$ concludes the proof of Theorem 7.1.7. □

It remains to prove Lemma 7.1.9. In the following, let $v \in l^p(\mathbb{Z})$ where $p \geq 1$. To begin, we recall (see (7.1.4)) that

$$(FJ_0 f)(\theta) = 2\cos(\theta)(Ff)(\theta), \quad f \in l^2(\mathbb{Z}), \quad \theta \in [0, 2\pi),$$

where F denotes the Fourier transform. Consequently, for $\lambda \in \mathbb{C} \setminus [-2,2]$ we have

$$R_{J_0}(\lambda) = F^{-1} M_{g_\lambda} F,$$

where $M_{g_\lambda} \in \mathcal{B}(L^2(0,2\pi))$ is the operator of multiplication by the bounded function

$$g_\lambda(\theta) = (\lambda - 2\cos(\theta))^{-1}, \quad \theta \in [0,2\pi). \tag{7.1.17}$$

Since $g_\lambda = |g_\lambda|^{1/2} \cdot \frac{g_\lambda}{|g_\lambda|} \cdot |g_\lambda|^{1/2}$, we can define the unitary operator

$$T = F^{-1} M_{g_\lambda/|g_\lambda|} F$$

to obtain the identity

$$\|UM_{v^{1/2}} R_{J_0}(\lambda) M_{v^{1/2}}\|_{\mathcal{S}_p}^p = \|UM_{v^{1/2}} F^{-1} M_{|g_\lambda|^{1/2}} F T F^{-1} M_{|g_\lambda|^{1/2}} F M_{v^{1/2}}\|_{\mathcal{S}_p}^p.$$

Using Hölder's inequality for Schatten norms (see Section 2.2), and recalling that $\|U\| \leq 3$, we thus obtain

$$\begin{aligned} \|UM_{v^{1/2}} R_{J_0}(\lambda) M_{v^{1/2}}\|_{\mathcal{S}_p}^p &\leq 3^p \|M_{v^{1/2}} F^{-1} M_{|g_\lambda|^{1/2}} F\|_{\mathcal{S}_{2p}}^p \|F^{-1} M_{|g_\lambda|^{1/2}} F M_{v^{1/2}}\|_{\mathcal{S}_{2p}}^p \\ &= 3^p \|M_{v^{1/2}} F^{-1} M_{|g_\lambda|^{1/2}} F\|_{\mathcal{S}_{2p}}^{2p}. \end{aligned} \tag{7.1.18}$$

For the last identity we used the selfadjointness of the bounded operators $M_{v^{1/2}}$ and $F^{-1} M_{|g_\lambda|^{1/2}} F$ and the fact that the Schatten norm of an operator and its adjoint coincide.

To derive an estimate on the Schatten norm on the right-hand side of (7.1.18), we will use the following lemma (see [28], Lemma 10). Here, as above, $M_u \in \mathcal{B}(l^2(\mathbb{Z}))$ and $M_h \in \mathcal{B}(L^2(0,2\pi))$ denote the operators of multiplication by a sequence $u = \{u_m\} \in l^\infty(\mathbb{Z})$ and a function $h \in L^\infty(0,2\pi)$, respectively.

Lemma 7.1.10. *Let $q \geq 2$ and suppose that $u = \{u_m\} \in l^q(\mathbb{Z})$ and $h \in L^\infty(0,2\pi)$. Then*

$$\|M_u F^{-1} M_h F\|_{\mathcal{S}_q} \leq (2\pi)^{-1/q} \|u\|_{l^q} \|h\|_{L^q}. \tag{7.1.19}$$

Remark 7.1.11. For operators on $L^2(\mathbb{R}^d)$ an analogous result is well known, see Lemma 7.2.8 below.

Since $p \geq 1$ (and so $2p \geq 2$), the previous lemma and (7.1.18) imply that

$$\|UM_{v^{1/2}}R_{J_0}(\lambda)M_{v^{1/2}}\|_{\mathcal{S}_p}^p \leq C(p)\|M_{v^{1/2}}F^{-1}M_{|g_\lambda|^{1/2}}F\|_{\mathcal{S}_{2p}}^{2p} \leq C(p)\|v\|_{l^p}^p\|g_\lambda\|_{L^p}^p. \tag{7.1.20}$$

The proof of Lemma 7.1.9 is completed by an application of the following result ([28], Lemma 9).

Lemma 7.1.12. *Let $\lambda \in \mathbb{C} \setminus [-2,2]$ and let $g_\lambda : [0,2\pi) \to \mathbb{C}$ be defined by* (7.1.17). *Then the following holds: If $p > 1$ then*

$$\|g_\lambda\|_{L^p}^p \leq \frac{C(p)}{\operatorname{dist}(\lambda,[-2,2])^{p-1}|\lambda^2-4|^{1/2}}. \tag{7.1.21}$$

Furthermore, for every $0 < \varepsilon < 1$ we have

$$\|g_\lambda\|_{L^1} \leq \frac{C(\varepsilon)}{\operatorname{dist}(\lambda,[-2,2])^{\varepsilon}|\lambda^2-4|^{(1-\varepsilon)/2}}. \tag{7.1.22}$$

Remark 7.1.13. In this section we have finally seen why it was advantageous to formulate Theorem 4.2.2 in terms of estimates on $M_2R_{A_0}(\lambda)M_1$ (see (4.2.3)) instead of estimates on $MR_{A_0}(\lambda)$ (where $A = A_0 + M = A_0 + M_1M_2$). Without this decomposition the estimates in Theorem 7.1.7 could have been proved for $p \geq 2$ only, due to the restriction to such p's in Lemma 7.1.10.

7.2. Schrödinger operators

In the following we consider Schrödinger operators $H = -\Delta + V$ in $L^2(\mathbb{R}^d)$, where $V \in L^p(\mathbb{R}^d)$ is a complex-valued potential with

$$\begin{aligned} &p \geq 1, \quad \text{if } d = 1\\ &p > 1, \quad \text{if } d = 2\\ &p \geq \tfrac{d}{2}, \quad \text{if } d \geq 3. \end{aligned} \tag{7.2.1}$$

More precisely, H is the unique m-sectorial operator associated to the closed, densely defined, sectorial form

$$\mathcal{E}(f,g) = \langle \nabla f, \nabla g\rangle + \langle Vf, g\rangle, \quad \operatorname{Dom}(\mathcal{E}) = W^{1,2}(\mathbb{R}^d).$$

In particular, there exists $\omega \leq 0$ and $\theta \in [0, \frac{\pi}{2})$ such that

$$\sigma(H) \subset \overline{\operatorname{Num}}(H) \subset \{\lambda : |\arg(\lambda - \omega)| \leq \theta\} \tag{7.2.2}$$

and so (2.1.11) implies that

$$\|R_H(\lambda)\| \leq |\operatorname{Re}(\lambda) - \omega|^{-1}, \qquad \operatorname{Re}(\lambda) < \omega. \tag{7.2.3}$$

Remark 7.2.1. We note that for $V \in L^p(\mathbb{R}^d)$ with $p \geq 2$ if $d \leq 3$ and $p > d/2$ if $d \geq 4$ the multiplication operator M_V, defined as

$$(M_Vf)(x) = V(x)f(x), \quad \operatorname{Dom}(M_V) = \{f \in L^2 : Vf \in L^2\},$$

is relatively compact with respect to $-\Delta$ (see Lemma 7.2.9), so in this case the operator H coincides with the usual operator sum $-\Delta + M_V$ defined on

$\mathrm{Dom}(-\Delta) = W^{2,2}(\mathbb{R}^d)$. Here, as usual, $-\Delta$ is defined via the Fourier transform F on L^2, i.e., $-\Delta = F^{-1}M_{|k|^2}F$.

It can be shown that the resolvent difference $(-a-H)^{-1} - (-a+\Delta)^{-1}$ is compact for $a > 0$ sufficiently large, so Corollary 2.3.3 implies that the spectrum of H consists of $[0,\infty) = \sigma(-\Delta)$ and a possible additional set of discrete eigenvalues which can accumulate at $[0,\infty)$ only. A classical result in the study of these isolated eigenvalues for *selfadjoint* Schrödinger operators are the Lieb–Thirring (L-T) inequalities, which state that for $V = \overline{V} \in L^p(\mathbb{R}^d)$ with p satisfying (7.2.1) one has

$$\sum_{\lambda \in \sigma_d(H), \lambda < 0} |\lambda|^{p-\frac{d}{2}} \leq C(p,d) \|V_-\|_{L^p}^p, \tag{7.2.4}$$

where $V_- = -\min(V,0)$ denotes the negative part of V. These inequalities were a major tool in Lieb and Thirring's proof of the stability of matter [36] and the search for the optimal constants $C(p,d)$ remains an active field of current research. We refer to [35, 29] for more information on these topics.

In recent times, starting with work of Abramov, Aslanyan and Davies [1], there has also been an increasing interest in analogs of the L-T-inequalities for non-selfadjoint Schrödinger operators. For instance, Frank, Laptev, Lieb and Seiringer [17] considered the eigenvalues in sectors avoiding the positive half-line. By reduction to a selfadjoint problem (essentially doing what was sketched in Remark 5.2.7) they showed that for $p \geq d/2+1$ and $\chi > 0$

$$\sum_{\lambda \in \sigma_d(H), |\operatorname{Im}(\lambda)| \geq \chi \operatorname{Re}(\lambda)} |\lambda|^{p-\frac{d}{2}} \leq C(p,d) \left(1 + \frac{2}{\chi}\right)^p \| \operatorname{Re}(V)_- + i \operatorname{Im}(V)\|_{L^p}^p. \tag{7.2.5}$$

Remark 7.2.2. By a suitable integration of inequality (7.2.5) one can obtain an estimate on all discrete eigenvalues of H, see Corollary 3 in [9]. We will not discuss this result in this review.

Concerning eigenvalues accumulating to $[0,\infty)$ Laptev and Safronov [34] proved the following result: If $\operatorname{Re}(V) \geq 0$ and $V \in L^p(\mathbb{R}^d)$ for $p \geq 1$ if $d = 1$ and $p > \frac{d}{2}$ if $d \geq 2$ then

$$\sum_{\lambda \in \sigma_d(H), \operatorname{Re}(\lambda) \geq 0} \left(\frac{|\operatorname{Im}(\lambda)|}{|\lambda+1|^2+1} \right)^p \leq C(p,d) \|\operatorname{Im}(V)\|_{L^p}^p. \tag{7.2.6}$$

Finally, let us also mention the recent work of Frank [16], which provides conditions for the boundedness of the eigenvalues of H outside $[0,\infty)$, and the related works of Safronov [41, 42].

Now let us have a look at what kind of L-T-inequalities we can obtain from Theorem 4.4.6 and 5.3.3, respectively, and how these inequalities will compare to each other and to the inequalities (7.2.5) and (7.2.6). We note that the results to follow can be regarded as refinements of our earlier work [9] (see also [25]).

We start with an application of Theorem 4.4.6, where we require the stronger assumption that M_V is $(-\Delta)$-compact (see Remark 7.2.1 above).

Theorem 7.2.3. *Let $H = -\Delta + V$ be defined as above and let $\omega \le 0$ be as defined in* (7.2.2)*. We assume that $V \in L^p(\mathbb{R}^d)$ with $p \ge 2$ if $d \le 3$ and $p > d/2$ if $d > 4$. Then for $\tau \in (0,1)$ the following holds:* (i) *If $\omega < 0$ and $p \ge d - \tau$ then*

$$\sum_{\lambda \in \sigma_d(H)} \frac{\operatorname{dist}(\lambda, [0,\infty))^{p+\tau}}{|\lambda|^{\frac{d}{2}}(|\lambda| + |\omega|)^{2\tau}} \le C(d,p,\tau)|\omega|^{-\tau}\|V\|_{L^p}^p. \tag{7.2.7}$$

(ii) *If $\omega < 0$ and $p < d - \tau$ then*

$$\sum_{\lambda \in \sigma_d(H)} \frac{\operatorname{dist}(\lambda, [0,\infty))^{p+\tau}}{|\lambda|^{\frac{p+\tau}{2}}(|\lambda| + |\omega|)^{\frac{d-p+3\tau}{2}}} \le C(d,p,\tau)|\omega|^{-\tau}\|V\|_{L^p}^p. \tag{7.2.8}$$

(iii) *If $\omega = 0$ then for $s > 0$*

$$\sum_{\lambda \in \sigma_d(H), |\lambda| > s} \frac{\operatorname{dist}(\lambda, [0,\infty))^{p+\tau}}{|\lambda|^{\frac{d}{2}+2\tau}} + \sum_{\lambda \in \sigma_d(H), |\lambda| \le s} \frac{\operatorname{dist}(\lambda, [0,\infty))^{p+\tau}}{|\lambda|^{\frac{d}{2}} s^{2\tau}} \le C(d,p,\tau)s^{-\tau}\|V\|_{L^p}^p. \tag{7.2.9}$$

Before presenting the proof of Theorem 7.2.3 let us consider what can be obtained by applying Theorem 5.3.3 in the present context. Here, as compared to Theorem 7.2.3, we don't need the relative compactness of M_V but can (almost) stick to the more general assumption (7.2.1). However, now we require that $\operatorname{Re}(V) \ge \omega$ for some $\omega \le 0$, which was not necessary in the previous result.

Remark 7.2.4. Note that $\operatorname{Re}(V) \ge \omega$ is a sufficient but *not* a necessary condition for $\operatorname{Num}(H)$ being a subset of $\{\lambda : \operatorname{Re}(\lambda) \ge \omega\}$.

Theorem 7.2.5. *Let $H = -\Delta + V$ be defined as above, where we assume that $V \in L^p(\mathbb{R}^d)$ with $p \ge 1$ if $d = 1$ and $p > d/2$ if $d \ge 2$. In addition, we assume that* $\operatorname{Re}(V) \ge \omega$ *for $\omega \le 0$. Then for $\tau > 0$ the following holds:*

(i) *If $\omega < 0$ then*

$$\sum_{\lambda \in \sigma_d(H)} \frac{\operatorname{dist}(\lambda, [0,\infty))^{p}}{(|\lambda| + |\omega|)^{\frac{d}{2}+\tau}} \le C(d,p,\tau)|\omega|^{-\tau}\|\operatorname{Re}(V)_- + i\operatorname{Im}(V)\|_{L^p}^p. \tag{7.2.10}$$

(ii) *If $\omega = 0$ then for $s > 0$*

$$\sum_{\substack{\lambda \in \sigma_d(H) \\ |\lambda| > s}} \frac{\operatorname{dist}(\lambda, [0,\infty))^{p}}{|\lambda|^{\frac{d}{2}+\tau}} + \sum_{\substack{\lambda \in \sigma_d(H) \\ |\lambda| \le s}} \frac{\operatorname{dist}(\lambda, [0,\infty))^{p}}{|\lambda|^{\frac{d}{2}-\tau} s^{2\tau}} \le Cs^{-\tau}\|\operatorname{Re}(V)_- + i\operatorname{Im}(V)\|_{L^p}^p, \tag{7.2.11}$$

where $C = C(d,p,\tau)$.

As the reader might already have guessed, the comparison of the estimates obtained in the previous two theorems and the estimates (7.2.5) and (7.2.6) is a quite complex task, requiring the analysis of a variety of different cases. However, we think it is better not to be too pedantic here, and so will restrict ourselves to a broad sketch of what is going on.

The first thing that is apparent is that the previous two theorems provide estimates which are not restricted to certain subsets of eigenvalues, as was the case with the estimates (7.2.5) and (7.2.6). Concerning the L^p-assumptions on V, Theorem 7.2.5 and estimate (7.2.6) are less restrictive than the other two results; on the other hand, both Theorem 7.2.5 and estimate (7.2.6) require an additional assumption on the real part of the potential. Concerning the right-hand sides of the inequalities, estimate (7.2.5) stands out, since it is the only estimate which depends on H only through the L^p-norm of the potential V, all other estimates also depending on $\omega = \omega(H)$. Whether this ω-dependence is indeed necessary if one is considering all eigenvalues of H, not restricting oneself to eigenvalues outside sectors, is one among the many open questions on this topic.

Concerning the amount of information on the discrete eigenvalues that can be obtained from the different results, one has to distinguish between sequences of eigenvalues converging to some point in $(0, \infty)$ and to 0, respectively, quite similarly to the case of Jacobi operators where we also had to distinguish between interior and boundary points of the essential spectrum. Suffice it to say that here, as in the Jacobi case, Theorem 7.2.3 (to be obtained via the complex analysis approach) is weaker than Theorem 7.2.5 (to be obtained via the operator-theory approach) concerning sequences of eigenvalues converging to some interior point of the essential spectrum $[0, \infty)$, whereas each of the results can be stronger than the other if one is considering eigenvalues converging to the boundary point 0, depending on the parameters involved.

Problem 7.2.6. *All of the above results seem to suggest that the most natural generalization of the selfadjoint L-T-inequalities to the non-selfadjoint setting would be an estimate of the form*

$$\sum_{\lambda \in \sigma_d(H)} \frac{\operatorname{dist}(\lambda, [0,\infty))^p}{|\lambda|^{\frac{d}{2}}} \leq C(p,d) \|V\|_{L^p}^p, \tag{7.2.12}$$

with p satisfying Assumption (7.2.1) (*this is particularly true of the above estimates in case that $\omega = 0$, just formally set $\tau = 0$*)*. The validity or falsehood of estimate* (7.2.12)*, without any additional assumptions on V, can justly be regarded as one of the major open problems in this field* (*see also* [10])*.*

It remains to present the proofs of Theorem 7.2.3 and Theorem 7.2.5. Both will rely on estimates on the $\mathcal{S}_p$-norm of operators of the form $M_W(\lambda + \Delta)^{-1}$. Since $(\lambda + \Delta)^{-1} = F^{-1} M_{k_\lambda} F$, where

$$k_\lambda(x) = (\lambda - |x|^2)^{-1}, \quad x \in \mathbb{R}^d, \tag{7.2.13}$$

as in the case of Jacobi operators this estimate will be reduced to an estimate on the L^p-norm of the bounded function k_λ. We will need the following three lemmas.

Lemma 7.2.7. *Let $d \geq 1$. Then for $\lambda \in \mathbb{C} \setminus [0, \infty)$ and k_λ as defined in* (7.2.13) *the following holds: If $p > \max(d/2, 1)$ then*

$$\|k_\lambda\|_{L^p}^p \leq C(p,d) \frac{|\lambda|^{\frac{d}{2}-1}}{\operatorname{dist}(\lambda, [0,\infty))^{p-1}}. \tag{7.2.14}$$

Proof. For the elementary but quite lengthy proof we refer to [25], page 103. □

The next result has already been hinted at in the study of Jacobi operators (see Lemma 7.1.10). See Simon [44], Theorem 4.1, for a proof.

Lemma 7.2.8. *Let $f, g \in L^p(\mathbb{R}^d)$ where $p \geq 2$. Then the operator $M_f F^{-1} M_g F$ is in $\mathcal{S}_p(L^2(\mathbb{R}^d))$ and*

$$\|M_f F^{-1} M_g F\|_{\mathcal{S}_p}^p \leq (2\pi)^{-d} \|f\|_{L^p}^p \|g\|_{L^p}^p.$$

Combining the previous two lemmas, we obtain a bound on the $\mathcal{S}_p$-norm of $M_W(\lambda + \Delta)^{-1}$.

Lemma 7.2.9. *Let $W \in L^p(\mathbb{R}^d)$ where $p \geq 2$ if $d \leq 3$ and $p > d/2$ if $d \geq 4$. Then for $\lambda \in \mathbb{C} \setminus [0, \infty)$ we have*

$$\|M_W(\lambda + \Delta)^{-1}\|_{\mathcal{S}_p}^p \leq C(p,d) \|W\|_{L^p}^p \frac{|\lambda|^{\frac{d}{2}-1}}{\operatorname{dist}(\lambda, [0,\infty))^{p-1}}. \tag{7.2.15}$$

We are now prepared for the

Proof of Theorem 7.2.3. We apply Theorem 4.4.6 with $H = -\Delta + M_V$ and $H_0 = -\Delta$, taking estimate (7.2.3) into account. With the notation of that theorem we obtain from the previous lemma that $\alpha = p - 1, \beta = \frac{d}{2} - 1, C_0 = 1$ and $K = C(p,d)\|V\|_{L^p}^p$. All that remains is to compute the constants η_0, η_1 and η_2 appearing in Theorem 4.4.6, treating the cases $p \geq d - \tau$ and $p < d - \tau$ separately (and noting that by assumption $\tau \in (0,1)$). □

The proof of Theorem 7.2.5 is a little more involved.

Proof of Theorem 7.2.5. First of all we note that using an approximation argument it is sufficient to prove the theorem assuming that $V \in L_0^\infty(\mathbb{R}^d)$, the bounded functions with compact support, see [26, Lemma 5.4] for more details. In particular, in this case $H = -\Delta + M_V$ since M_V is $(-\Delta)$-compact.

So in the following let $V \in L_0^\infty(\mathbb{R}^d)$ with $\operatorname{Re}(V) \geq \omega$ ($\omega \leq 0$) and let $H = -\Delta + M_V$ and $H_0 = -\Delta + M_{\operatorname{Re}(V)_+}$. We are going to show that for $a < \omega$ and $p \geq 1$ if $d = 1$ or $p > \frac{d}{2}$ if $d \geq 2$ we have

$$\|R_H(a) - R_{H_0}(a)\|_{\mathcal{S}_p}^p \leq C(p,d) \frac{1}{|a|^{p-\frac{d}{2}}(|a| - |\omega|)^p} \|\operatorname{Re}(V)_- + i \operatorname{Im}(V)\|_p^p. \tag{7.2.16}$$

If this is done an application of Theorem 5.3.3 will conclude the proof.

As a first step in the proof of (7.2.16) we use the second resolvent identity to rewrite the resolvent difference as

$$R_H(a) - R_{H_0}(a) = (a-H)^{-1}(-a-\Delta)^{1/2}(-a-\Delta)^{-1/2}M_{|W|^{1/2}}M_{\mathrm{sign}(W)}$$
$$M_{|W|^{1/2}}(-a-\Delta)^{-1/2}(-a-\Delta)^{1/2}(a-H_0)^{-1},$$

where

$$W = -\mathrm{Re}(V)_- + i\,\mathrm{Im}(V) \quad \text{and} \quad \mathrm{sign}(W) = W/|W|.$$

Note that $-\Delta - a \geq -a \geq 0$. We will show below that $(-a-\Delta)^{1/2}(a-H_0)^{-1}$ is bounded on $L^2(\mathbb{R}^d)$ with

$$\|(-a-\Delta)^{1/2}(a-H_0)^{-1}\| \leq |a|^{-1/2}. \tag{7.2.17}$$

Moreover, we will show that for the closure of $(a+H)^{-1}(a-\Delta)^{1/2}$, initially defined on $\mathrm{Dom}((-\Delta)^{1/2}) = W^{1,2}(\mathbb{R}^d)$, we have

$$\|\overline{(a-H)^{-1}(-a-\Delta)^{1/2}}\| \leq \frac{|a|^{1/2}}{|a|-|\omega|}. \tag{7.2.18}$$

Hence, using Hölder's inequality for Schatten norms, the unitarity of $M_{\mathrm{sign}(W)}$ and the fact that the Schatten norm of an operator and its adjoint coincide we obtain

$$\begin{aligned}
&\|R_H(a) - R_{H_0}(a)\|_{\mathcal{S}_p}^p \\
&\quad\leq (|a|-|\omega|)^{-p}\|(-a-\Delta)^{-1/2}M_{|W|^{1/2}}M_{\mathrm{sign}(W)}M_{|W|^{1/2}}(-a-\Delta)^{-1/2}\|_{\mathcal{S}_p}^p \\
&\quad\leq (|a|-|\omega|)^{-p}\|M_{|W|^{1/2}}(-a-\Delta)^{-1/2}\|_{\mathcal{S}_{2p}}^{2p}.
\end{aligned} \tag{7.2.19}$$

Since $p \geq 1$ and $p > d/2$ we can then apply Lemma 7.2.8 and Lemma 7.2.7 to obtain

$$\begin{aligned}
\|M_{|W|^{1/2}}(-a-\Delta)^{-1/2}\|_{\mathcal{S}_{2p}}^{2p} &= \|M_{|W|^{1/2}}F^{-1}|k_a|^{1/2}F\|_{\mathcal{S}_{2p}}^{2p} \\
&\leq (2\pi)^{-d}\|W\|_{L^p}^p\|k_a\|_{L^p}^p \leq C(p,d)\|W\|_{L^p}^p|a|^{d/2-p}.
\end{aligned} \tag{7.2.20}$$

Remark 7.2.10. The validity of the last estimate for $p = 1$ and $d = 1$ (which is not contained in Lemma 7.2.7) is easily established.

The estimates (7.2.19) and (7.2.20) show the validity of (7.2.16). It remains to prove (7.2.17) and (7.2.18). To prove (7.2.18), let $f \in L^2(\mathbb{R}^d)$ with $\|f\| = 1$. Then

$$\begin{aligned}
&\|(-a-\Delta)^{1/2}(a-H^*)^{-1}f\|^2 \\
&\quad= -\langle f, (a-H^*)^{-1}f\rangle - \langle \overline{V}(a-H^*)^{-1}f, (a-H^*)^{-1}f\rangle.
\end{aligned}$$

Since $\mathrm{Re}(V) \geq \omega$ we obtain

$$\begin{aligned}
&\|(-a-\Delta)^{1/2}(a-H^*)^{-1}f\|^2 \\
&\quad = -\mathrm{Re}(\langle f, (a-H^*)^{-1}f\rangle) - \mathrm{Re}(\langle \overline{V}(a-H^*)^{-1}f, (a-H^*)^{-1}f\rangle) \\
&\quad \leq -\mathrm{Re}(\langle f, (a-H^*)^{-1}f\rangle) + |\omega|\|(a-H^*)^{-1}f\|^2 \\
&\quad \leq \|(a-H^*)^{-1}\| + |\omega|\|(a-H^*)^{-1}\|^2 \\
&\quad \leq \frac{1}{\mathrm{dist}(a, \overline{\mathrm{Num}}(H^*))} + \frac{|\omega|}{\mathrm{dist}(a, \overline{\mathrm{Num}}(H^*))^2} \\
&\quad \leq \frac{1}{|a|-|\omega|} + \frac{|\omega|}{(|a|-|\omega|)^2} = \frac{|a|}{(|a|-|\omega|)^2}. \qquad (7.2.21)
\end{aligned}$$

But (7.2.21) implies (7.2.18) since

$$\overline{(a-H)^{-1}(-a-\Delta)^{1/2}} = [(-a-\Delta)^{1/2}(a-H^*)^{-1}]^*.$$

The proof of (7.2.17) is similar (and even simpler) and is therefore omitted. □

8. An outlook

In this final section we would like to present a short list of possible extensions of the results discussed in this paper, and of some open problems connected to these results which we think might be worthwhile to pursue.

1. The majority of results in this paper dealt with non-selfadjoint perturbations of selfadjoint operators, with a particular emphasis on the case where the spectrum of the unperturbed operator is an interval. This choice of operators was sufficient for the applications we had in mind, but there are also two more intrinsic reasons for this restriction. Namely, in this case the closure of the numerical range and the spectrum of the unperturbed operator coincide, which was necessary for a suitable application of the operator-theoretic approach. Moreover, given this restriction the (extended) resolvent set of the unperturbed operator is conformally equivalent to the unit disk, which was important for the complex analysis approach.

   Recent developments suggest that the restriction to such operators is not really necessary and that both our methods can be applied in a much wider context. Concerning the operator-theory approach this is a consequence of the fact that estimate (5.1.3) remains valid (for $p > 1$) for arbitrary perturbations of selfadjoint operators (see [27]), without any restriction on the spectrum of the selfadjoint operator (i.e., it does not need to be an interval). Concerning the complex analysis approach it follows from the fact that our main tool, the result of Borichev, Golinskii and Kupin (Theorem 3.3.1) has been generalized to functions acting on finitely connected [23] and more general domains [15]. These new results will allow to analyze a variety of interesting operators (like, e.g., periodic Schrödinger operators perturbed by complex potentials), and they also lead to the question of the ultimate limits of applicability of our methods.

2. We have seen that neither of the two methods for studying eigenvalues developed in this paper subsumes the other, in the sense that each method allows us to prove some results which cannot, at least at the present stage of our knowledge, be obtained from the other. One may thus wonder whether there is some 'higher' viewpoint from which one could obtain all the results which are derived by the two methods. Since our two methods seem to rely on different ideas, it is not at all clear what such a generalized approach would look like.
3. In Chapter 7 we have applied our results to Jacobi and Schrödinger operators. Many opportunities exist for applying the results to other concrete classes of operators, e.g., Jacobi-type operators in higher dimensions, systems of partial differential equations, composition operators and so on. Each application might involve its own technical challenges, which might be interesting in themselves.
4. Many questions remain as to the optimality or sharpness of our results. Such questions are, of course, relative to the precise class of operators considered, and we refer particularly to Problem 7.1.8 regarding Jacobi operators and to Problem 7.2.6 regarding Schrödinger operators. Moreover the question of optimality can be understood in two senses. In the narrow sense, for a particular inequality we want to know that it cannot be strengthened with respect to the values of the exponents appearing in it. To obtain this it is sufficient to construct a single operator for which the distribution of eigenvalues is exactly as implied by the inequality, and no better. In a wider (and much more difficult) sense, one would like to know whether some inequalities completely characterize the possible set of eigenvalues of operators of a particular class of operators. To show this, one must construct, for *each* set of complex numbers satisfying the inequality, an operator in the relevant class which has precisely this set of eigenvalues – that is solve an inverse problem. Techniques for constructing operators of certain classes with explicitly known spectrum would thus be very valuable.
5. Another direction which should be interesting and challenging is the generalization of results of the type considered here to operators on Banach spaces. The notions of Schatten-class perturbations, of infinite determinants and of the numerical range, which are all central for us, have generalizations to Banach spaces, so that one can hope that at least some of our results can be generalized. This might lead to further information on concrete classes of operators.
6. It should be mentioned that in spectral theory and its applications, the distribution of eigenvalues is only one aspect of interest, and one would also like to learn about the corresponding eigenvectors. In the case of non-selfadjoint operators, the eigenvectors are not orthogonal, and we do not have the spectral theorem which ensures that the Hilbert space is a direct sum of subspaces

corresponding to the discrete and the essential spectrum. We would like to know more about the eigenvectors and the subspace generated by them.

7. A related direction somewhat removed from our work, but with which potential connections could be made, is the numerical computation of eigenvalues of operators of the type that have been considered here. How should one go about in obtaining approximations of eigenvalues of non-selfadjoint operators which are relatively compact perturbations of an operator with essential spectrum, and can some of the ideas used in our investigations (e.g., the perturbation determinant and complex analysis) be of use in the development of effective algorithms and/or in their analysis?

List of important symbols

$(.)_\pm$ – positive and negative part of a function/number
$\langle .,. \rangle$ – scalar product
$\mathcal{B}(\mathcal{H})$ – bounded linear operators on $\mathcal{H}$
$\mathcal{C}(\mathcal{H})$ – closed linear operators in $\mathcal{H}$
$\hat{\mathbb{C}}$ – extended complex plane
$\mathbb{D}$ – unit disk in the complex plane
$d_a, d_a^{Z,Z_0}, d_\infty, d_\infty^{Z,Z_0}$ – perturbation determinants (Section 2.4)
Dom(.) – domain of an operator/form
$(-\Delta)$ – Laplace operator in $L^2(\mathbb{R}^d)$
$\mathcal{H}$ – a complex separable Hilbert space
$H(\mathbb{D})$ – holomorphic functions in the unit disk
Ker(.) – kernel of a linear operator
M_V, M_v – operator of multiplication by V, v in $L^2(\mathbb{R}^d), l^2(\mathbb{Z})$
$\mathcal{M}, \mathcal{M}(\alpha, \vec{\beta}, \gamma, \vec{\xi}, K)$ – subclass of $H(\mathbb{D})$ (see Definition 3.1.1)
$N(h,r)$ – number of zeros of $h \in H(\mathbb{D})$ in the closed disk of radius r around the origin
$\|.\|_{\mathcal{S}_p}$ – Schatten-p-norm
Num(.) – numerical range of a linear operator
$P_Z, P_Z(\lambda)$ – Riesz projection
Ran(.) – range of a linear operator
Rank(.) – rank of a linear operator
$R_Z(\lambda) = (\lambda - Z)^{-1}$ – the resolvent
$\mathbb{R}_+$ – the interval $[0,\infty)$
$\rho(.), \hat{\rho}(.)$ – (extended) resolvent set of a linear operator
$\mathcal{S}_\infty(\mathcal{H})$ – compact linear operators on $\mathcal{H}$
$\mathcal{S}_p(\mathcal{H})$ – Schatten class of order p
$\sigma(.), \sigma_d(.), \sigma_{\mathrm{ess}}(.)$ – spectrum (discrete, essential) of a linear operator
$\mathbb{T}$ – unit circle in the complex plane
$(\mathbb{T}^N)_*$ – subset of $\mathbb{T}^N$ (see Definition 3.1.7)
$\dot{\cup}$ – a disjoint union
$\mathcal{Z}(.)$ – zero set of a function

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Solvable Models of Resonances and Decays

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Abstract. Resonance and decay phenomena are ubiquitous in the quantum world. To understand them in their complexity it is useful to study solvable models in a wide sense, that is, systems which can be treated by analytical means. The present review offers a survey of such models starting the classical Friedrichs result and carrying further to recent developments in the theory of quantum graphs. Our attention concentrates on dynamical mechanism underlying resonance effects and at time evolution of the related unstable systems.

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1. Introduction

Any general physical theory deals not only with objects as they are but also has to ask how they emerge and disappear in the time evolution and what one can learn from their temporary existence. In the quantum realm such processes are even more important than in classical physics. With few notable exceptions the elementary particles are unstable and also among nuclei, atoms and molecules unstable systems widely outnumber stable ones, even if the lack of permanence is a relative notion – it is enough to recall that the observed lifetime scale of particles and nuclei ranges from femtoseconds to geological times.

It is natural that the quantum theory had to deal with such temporarily existent objects already in its nascent period, and it did it using simple means suggested by the intuition of the founding fathers. As time went, of course, a need appeared for a better understanding of these phenomena even if there was no substantial doubt about their mechanism; one can cite, e.g., a critical discussion of the textbook derivation of the 'Fermi golden rule' [Fe, lecture 23] in [RS, notes to

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Sec. XII.6], or the necessarily non-exponential character of decay laws [Ex, notes to Sec. I.3] which surprisingly keeps to puzzle some people to this day.

The quest for mathematically consistent description of resonance effects brought many results. It is worth to mention that some of them were rather practical. Maybe the best example of the last claim is the method of determining resonance poles using the so-called complex scaling. It has distinctively mathematical roots, in particular, in the papers [AC71, BC71, Si79], however, its applications in molecular physics were so successful that people in this area refer typically to secondary sources such as [Mo98] instead giving credit to the original authors.

Description of resonances and unstable system dynamics is a rich subject with many aspects. To grasp them in their full complexity it is useful to develop a variety of tools among which an important place belongs to various solvable models of such systems. Those are the main topic of the present review paper which summarizes results obtained in this area over a long time period by various people including the author and his collaborators. As a *caveat*, however, one has say also that the subject has so many aspects that a review like this one cannot cover all of them; our ambition is to give just a reasonably complete picture. We also remain for the moment vague about what the adjective 'solvable' could mean in the present context; we will return to this question in Section 5 below. Finally, as it is customary in a review paper we will not give full proofs of the claims made; we typically sketch arguments leading to a described conclusion and we always provide a reference to the source where the full information can be found.

2. Preliminaries

Before starting the review it is useful to recall some notions we will need frequently in the following. Let us start with *resonances.* While from the physics point of view we usually have in mind a single phenomenon when speaking of a resonance in a quantum system, mathematically it may refer to different concepts.

We will describe two most important definitions starting from that of a *resolvent resonance.* A conservative quantum system is characterized by a family of observables represented by self-adjoint operators on an appropriate state Hilbert space. A prominent role among them is played by its Hamiltonian H, or operator of total energy. As a self-adjoint operator it has the spectrum which is a subset of the real line while the rest of the complex plane belongs to its resolvent set $\varrho(H)$ and the resolvent $z \mapsto (H-z)^{-1}$ is an analytic function on it having thus no singularities. It may happen, however, that it has an analytic continuation, typically across the cut given by the continuous spectrum of H – one usually speaks in this connection about another sheet of the 'energy surface' – and that this continuation is meromorhic having pole singularities which we identify with resonances.

An alternative concept is to associate resonances with scattering. Given a pair (H, H_0) of self-adjoint operators regarded as the full and free Hamiltonian of the system we can construct scattering theory in the standard way [AJS, RS], in particular, we can check existence of the scattering operator and demonstrate that it can be written in the form of a direct integral, the corresponding fiber operators being called *on-shell scattering matrices*. The latter can be extended to meromorhic function and resonances are identified in this case with their poles.

While the resonances defined in the two above-described ways often coincide, especially in the situations when $H = -\Delta + V$ is a Schrödinger operator and $H_0 = -\Delta$ its free counterpart, there is no *a priori* reason why it should be always true; it is enough to realize that resolvent resonances characterize a single operator while the scattering ones are given by a pair of them. Establishing equivalence between the two notions is usually one of the first tasks when investigating resonances.

In order to explain how resonances are related to temporarily existing objects we have to recall basic facts about unstable quantum systems. To describe such a system we must not regard it as isolated, rather as a part of a larger system including its decay products. We associated with the latter a state space $\mathcal{H}$ on which unitary evolution operator $U:\, U(t) = \mathrm{e}^{-iHt}$ related to a self-adjoint Hamiltonian H acts. The unstable system corresponds to a proper subspace $\mathcal{H}_{\mathrm{u}} \subset \mathcal{H}$ associated with a projection E_{u}. To get a nontrivial model we assume that $\mathcal{H}_{\mathrm{u}}$ is not invariant w.r.t. $U(t)$ for any $t > 0$; in that case we have $\|E_{\mathrm{u}}U(t)\psi\| < \|\psi\|$ for $\psi \in \mathcal{H}_{\mathrm{u}}$ and the state which is at the initial instant $t = 0$ represented by the vector ψ evolves into a superposition containing a component in $\mathcal{H}_{\mathrm{u}}^{\perp}$ describing the decay products. Evolution of the unstable system alone is determined by the *reduced propagator*

$$V:\ V(t) = E_{\mathrm{u}}U(t) \upharpoonright \mathcal{H}_{\mathrm{u}}\,,$$

which is a contraction satisfying $V(t)^* = V(-t)$ for any $t \in \mathbb{R}$, strongly continuous with respect to the time variable. For a unit vector $\psi \in \mathcal{H}_{\mathrm{u}}$ the *decay law*

$$P_\psi:\ P_\psi(t) = \|V(t)\psi\|^2 = \|E_{\mathrm{u}}U(t)\psi\|^2 \tag{2.1}$$

is a continuous function such that $0 \le P_\psi(t) \le P_\psi(0) = 1$ meaning the probability that the system undisturbed by measurement will be found undecayed at time t.

Under our assumptions the reduced evolution cannot be a group, however, it is not excluded that it has the semigroup property, $V(s)V(t) = V(s+t)$ for all $s, t \ge 0$. As a example consider the situation where $\mathcal{H}_{\mathrm{u}}$ is one-dimensional being spanned by a unit vector $\psi \in \mathcal{H}$ and the reduced propagator is a multiplication by

$$v(t) := (\psi, U(t)\psi) = \int_{\mathbb{R}} \mathrm{e}^{-i\lambda t} \mathrm{d}(\psi, E_\lambda^H \psi)\,,$$

where $E_\lambda^H = E_H(-\infty, \lambda]$ is the spectral projection of H. If ψ and H are such that the measure has Breit-Wigner shape, $\mathrm{d}(\psi, E_\lambda^H \psi) = \frac{\Gamma}{2\pi}\left[(\lambda - \lambda_0)^2 + \frac{1}{4}\Gamma^2\right]^{-1} \mathrm{d}\lambda$ for some $\lambda_0 \in \mathbb{R}$ and $\Gamma > 0$, we get $v(t) = \mathrm{e}^{-i\lambda_0 t - \Gamma|t|/2}$ giving exponential decay law. Note that the indicated choice of the measure requires $\sigma(H) = \mathbb{R}$; this conclusion is not restricted to the one-dimensional case but it holds generally.

Theorem 2.1 ([Si72]). *Under the stated assumptions the reduced propagator can have the semigroup property only if* $\sigma(H) = \mathbb{R}$.

At a glance, this seems to be a problem since the exponential character of the decay laws conforms with experimental evidence in most cases, and at the same time Hamiltonians are usually supposed to be below bounded. However, such a spectral restriction excludes only the *exact* validity of semigroup reduced evolution allowing it to be an approximation, possibly a rather good one. To understand better its nature, let us express the reduced evolution by means of the *reduced resolvent*, $R_H^{\mathrm{u}}(z) := E_{\mathrm{u}} R_H(z) \upharpoonright \mathcal{H}_{\mathrm{u}}$. Using the spectral decomposition of H we can write the reduced propagator as Fourier image,

$$V(t)\psi = \int_{\mathbb{R}} \mathrm{e}^{-i\lambda t} \mathrm{d}F_\lambda \psi \tag{2.2}$$

for any $\psi \in \mathcal{H}_{\mathrm{u}}$, of the operator-valued measure on $\mathbb{R}$ determined by the relation $F(-\infty, \lambda] := E_{\mathrm{u}} E_\lambda^{(H)} \upharpoonright \mathcal{H}_{\mathrm{u}}$. By the Stone formula, we can express the measure as

$$\frac{1}{2}\big\{F[\lambda_1, \lambda_2] + F(\lambda_1, \lambda_2)\big\} \;=\; \frac{1}{2\pi i} \operatorname*{s-lim}_{\eta\to 0+} \int_{\lambda_1}^{\lambda_2} \big[R_H^{\mathrm{u}}(\xi + i\eta) - R_H^{\mathrm{u}}(\xi - i\eta)\big]\, \mathrm{d}\xi\,;$$

the formula simplifies if the spectrum is purely absolutely continuous and the left-hand side can be simply written as $F(\lambda_1, \lambda_2)$.

The support of $F(\cdot)\psi$ is obviously contained in the spectrum of H and the same is true for $\operatorname{supp} F = \bigcup_{\psi\in\mathcal{H}_{\mathrm{u}}} \operatorname{supp} F(\cdot)\psi$, if fact, the latter coincides with $\sigma(H)$ [Ex76].

In view of that the reduced resolvent makes no sense at the points $\xi \in \operatorname{supp} F$ but the limits $\operatorname{s-lim}_{\eta\to 0+} R_H^{\mathrm{u}}(\xi \pm i\eta)$ may exist; if they are bounded on the interval (λ_1, λ_2) we may interchange the limit with the integral. Furthermore, since the resolvent is analytic in $\rho(H) = \mathbb{C} \setminus \sigma(H)$ the same is true for $R_H^{\mathrm{u}}(\cdot)$. At the points of $\operatorname{supp} F$ it has a singularity but it may have an *analytic continuation* across it; the situation is particularly interesting when this continuation has a meromorphic structure, i.e., isolated poles in the lower half-plane. For the sake of simplicity consider again the situation with $\dim \mathcal{H}_{\mathrm{u}} = 1$ when the reduced resolvent acts as a multiplication by $r_H^{\mathrm{u}}(z)$ and suppose its continuation has a single pole,

$$r_H^{\mathrm{u}}(z) = \frac{A}{z_{\mathrm{p}} - z} + f(z) \tag{2.3}$$

for $\operatorname{Im} z > 0$, where $A \neq 0$, f is holomorphic, and $z_{\mathrm{p}} := \lambda_{\mathrm{p}} - i\delta_{\mathrm{p}}$ is a point in the lower half-plane. Since $r_H^{\mathrm{u}}(\lambda - i\eta) = \overline{r_H^{\mathrm{u}}(\lambda + i\eta)}$, the measure in question is

$$\mathrm{d}F_\lambda = \frac{A}{2\pi i}\left(\frac{1}{\lambda - \overline{z}_{\mathrm{p}}} - \frac{1}{\lambda - z_{\mathrm{p}}}\right) \mathrm{d}\lambda + \frac{1}{\pi} \operatorname{Im} f(\lambda)\, \mathrm{d}\lambda\,,$$

and evaluating the reduced propagator using the residue theorem we get

$$v(t) = A\, \mathrm{e}^{-i\lambda_{\mathrm{p}} t - \delta_{\mathrm{p}}|t|} + \frac{1}{\pi} \int_{\mathbb{R}} \mathrm{e}^{-i\lambda t} \operatorname{Im} f(\lambda)\, d\lambda\,, \tag{2.4}$$

which is close to a semigroup, giving an approximately exponential decay law with $\Gamma = 2\delta_{\mathrm{p}}$, if the second term is small and A does not differ much from one. At the same time, the presence of the pole in the analytic continuation provides a link to the concept of (resolvent) resonance quoted above.

The main question in investigation of resonances and decays is to analyze how such singularities can arise from the dynamics of the systems involved. A discussion of this question in a variety of models will be our main topic in the following sections.

3. A progenitor: Friedrichs model

We start with the *mother of all resonance models* for which we are indebted to Kurt O. Friedrichs who formulated it in his seminal paper [Fr48]. This is not to say it was recognized as seminal immediately, quite the contrary. Only after T.D. Lee six years later came with a caricature model of decay in quantum field theory, it was slowly recognized that its essence was already analyzed by Friedrichs; references to an early work on the model can be found in [Ex, notes to Sec. 3.2].

The model exists in numerous modifications; we describe here the simplest one. We suppose that the state Hilbert space of the system has the form $\mathcal{H} := \mathbb{C} \oplus L^2(\mathbb{R}^+)$ where the one-dimensional subspace is identified with the space $\mathcal{H}_\mathrm{u}$ mentioned above; the states are thus described by the pairs $\binom{\alpha}{f}$ with $\alpha \in \mathbb{C}$ and $f \in L^2(\mathbb{R}^+)$. The Hamiltonian is the self-adjoint operator on $\mathcal{H}$, or rather the family of self-adjoint operators labelled by the *coupling constant* $g \in \mathbb{R}$, defined by

$$H_g = H_0 + gV\,, \quad H_g \binom{\alpha}{f} := \begin{pmatrix} \lambda_0 \alpha & g(v,f) \\ g\alpha v & Qf \end{pmatrix}, \tag{3.1}$$

where λ_0 is a positive parameter, $v \in L^2(\mathbb{R}^+)$ is sometimes called *form factor*, and Q is the operator of multiplication, $(Qf)(\xi) = \xi f(\xi)$. This in particular means that the continuous spectrum of H_0 covers the positive real axis and the eigenvalue λ_0 is embedded in it; one expects that the perturbation gV can move the corresponding resolvent pole from the real axis to the complex plane.

To see that it is indeed the case we have to find the reduced resolvent. The model is solvable in view of the *Friedrichs condition*, $E_\mathrm{d} V E_\mathrm{d} = 0$ where E_d is the projection to $\mathcal{H}_\mathrm{d} := L^2(\mathbb{R}^+)$, which means that the continuum states do not interact mutually. Using the second resolvent formula and the commutativity of operators E_u and $R_{H_0}(z)$ together with $E_\mathrm{u} + E_\mathrm{d} = I$ we can write $E_\mathrm{u} R_{H_g}(z) E_\mathrm{u}$ as

$$E_\mathrm{u} R_{H_0}(z) E_\mathrm{u} - gE_\mathrm{u} R_{H_0}(z) E_\mathrm{u} V E_\mathrm{u} R_{H_g}(z) E_\mathrm{u} - gE_\mathrm{u} R_{H_0}(z) E_\mathrm{u} V E_\mathrm{d} R_{H_g}(z) E_\mathrm{u}\,;$$

in a similar way we can express the ‘off-diagonal’ part of the resolvent as

$$E_\mathrm{d} R_{H_g}(z) E_\mathrm{u} = -gE_\mathrm{d} R_{H_0}(z) E_\mathrm{d} V E_\mathrm{u} R_{H_g}(z) E_\mathrm{u}\,,$$

where we have also employed the Friedrichs condition. Substituting from the last relation to the previous one and using $(H_0 - z) E_\mathrm{u} R_{H_0}(z) = E_\mathrm{u}$ together with the explicit form of the operators H_0, V, we find that $R^\mathrm{u}_{H_g}(z)$ acts for $\mathrm{Im}\, z \neq 0$ on

$\mathcal{H}_\mathrm{u} = \mathbb{C}$ as multiplication by the function

$$r_g^\mathrm{u} : \, r_g^\mathrm{u}(z) := \left(-z + \lambda_0 + g^2 \int_0^\infty \frac{|v(\lambda)|^2}{z-\lambda} \, \mathrm{d}\lambda \right)^{-1} . \tag{3.2}$$

To make use of this result we need an assumption about the form factor, for instance

(a) there is an entire $f : \mathbb{C} \to \mathbb{C}$ such that $|v(\lambda)|^2 = f(\lambda)$ holds for all $\lambda \in (0, \infty)$;

for the sake of notational simplicity one usually writes $f(z) = |v(z)|^2$ for nonreal z too keeping in mind that it is a complex quantity. This allows us to construct analytic continuation of $r_g^\mathrm{u}(\cdot)$ over $\sigma_\mathrm{c}(H_g) = \mathbb{R}^+$ to the lower complex half-plane in the form $r(z) = [-z + w(z,g)]^{-1}$, where

$$\begin{aligned} w(\lambda, g) &:= \lambda_0 + g^2 I(\lambda) - \pi i g^2 |v(\lambda)|^2 \quad \dots \quad \lambda > 0 \\ w(z,g) &:= \lambda_0 + g^2 \int_0^\infty \frac{|v(\xi)|^2}{z-\xi} \, \mathrm{d}\xi - 2\pi i g^2 |v(z)|^2 \quad \dots \quad \mathrm{Im}\, z < 0 \end{aligned} \tag{3.3}$$

and $I(\lambda)$ is defined as the principal value of the integral,

$$I(\lambda) := \mathcal{P} \int_0^\infty \frac{|v(\xi)|^2}{\lambda - \xi} \, \mathrm{d}\xi \; := \lim_{\varepsilon \to 0+} \left(\int_0^{\lambda-\varepsilon} + \int_{\lambda+\varepsilon}^\infty \right) \frac{|v(\xi)|^2}{\lambda-\xi} \, \mathrm{d}\xi \, ;$$

the analyticity can be checked using the edge-of-the-wedge theorem.

These properties of the reduced resolvent make it possible to prove the meromorphic structure of its analytic continuation. Resonances in the model are then given by zeros of the function $z \mapsto w(z,g) - z$. An argument using the implicit-function theorem [Ex, Sec. 3.2] leads to the following conclusion:

Theorem 3.1. *Assume* (a) *and* $v(\lambda_0) \neq 0$, *then* $r(\cdot)$ *has for all sufficiently small* $|g|$ *exactly one simple pole* $z_\mathrm{p}(g) := \lambda_\mathrm{p}(g) - i\delta_\mathrm{p}(g)$. *The function* $z_\mathrm{p}(\cdot)$ *is infinitely differentiable and the expansions*

$$\lambda_P(g) = \lambda_0 + g^2 I(\lambda_0) + \mathcal{O}(g^4) \, , \quad \delta_\mathrm{p}(g) = \pi g^2 |v(\lambda_0)|^2 + \mathcal{O}(g^4) \, , \tag{3.4}$$

are valid in the vicinity of the point $g = 0$ *referring to the unperturbed Hamiltonian.*

To summarize the above reasoning we have seen that resonance poles can arise from perturbation of eigenvalues embedded in the continuous spectrum and that, at least locally, their distance from the real axis is the smaller the weaker is the perturbation. Moreover, one observes here the phenomenon called *spectral concentration*: it is not difficult to check that the spectral projections of H_g to the intervals $I_g := (\lambda_0 - \beta g, \lambda_0 - \beta g)$ with a fixed $\beta > 0$ satisfy the relation

$$\mathrm{s}\text{-}\lim_{g \to 0} E_{H_g}(I_g) = E_\mathrm{u} \, .$$

Friedrichs model also allows us to illustrate other typical features of resonant systems. We have mentioned already the deep insight contained in the *Fermi golden* *rule*, which in the present context can be written as

$$\Gamma_{\mathrm{F}}(g) = 2\pi g^2 \, \frac{d}{d\lambda} \, \Big(V\psi_{\mathrm{u}}, E_\lambda^{(0)} P_c(H_0) V\psi_{\mathrm{u}} \Big) \Big|_{\lambda=\lambda_0} \,,$$

where $\{E_\lambda^{(0)}\}$ is the spectral decomposition of H_0 and $P_{\mathrm{c}}(H_0)$ the projection to the continuous spectral subspace of this operator. To realize that this is indeed what we know from quantum-mechanical textbooks, it is enough to realize that we use the convention $\hbar = 1$ and formally it holds $\frac{\mathrm{d}}{\mathrm{d}\lambda} E_\lambda^{(0)} P_{\mathrm{c}}(H_0) = |\lambda\rangle\langle\lambda|$. Using the explicit form of the operators involved we find

$$\Gamma_{\mathrm{F}}(g) = 2\pi g^2 \, \frac{d}{d\lambda} \int_0^\lambda |v(\xi)|^2 \, d\xi \, \Big|_{\lambda=\lambda_0} = 2\pi g^2 \, |v(\lambda_0)|^2 \,,$$

which is nothing else than the first nonzero term in the Taylor expansion (3.4). On the other hand, a formal use of the rule may turn its gold into brass: a warning example concerning the situation when the unperturbed eigenvalue is situated at the threshold of $\sigma_{\mathrm{c}}(H_0)$ is due to J. Howland [Ho74], see also [Ex, Example 3.2.5]. Recent analysis of near-threshold effects in a generalized Friedrichs model together with a rich bibliography can be found in [DJN11].

Resonances discussed so far have been resolvent resonances. One can also consider the pair (H_g, H_0) as a scattering system. Existence and completeness of the wave operators is easy to establish since the perturbation gV has rank two. What we are interested in is the on-shell S-matrix: if v is piecewise continuous and bounded in $\mathbb{R}^+$ one can check [Ex, Prop. 3.2.6] that it acts as multiplication by

$$S(\lambda) = 1 + 2\pi i g^2 \lim_{\epsilon\to 0+} |v(\lambda)|^2 \, r_g^{\mathrm{u}}(\lambda + i\epsilon) \,.$$

If v satisfies in addition the assumption (a) above, the function $S(\cdot)$ can be analytically continued across $\mathbb{R}^+$. It is obvious that if such a continuation has a pole at a point z_{p} of the lower complex half-plane, the same is true for $r_g^{\mathrm{u}}(\cdot)$, on the other hand, it may happen that a resolvent resonance is not a scattering resonance, namely if the continuation of $|v(\cdot)|^2$ has a zero at the point z_{p}.

Finally, the model can also describe a decaying system if we suppose that at the initial instant $t = 0$ the state is described by the vector $\binom{1}{0}$ which span the one-dimensional subspace $\mathcal{H}_{\mathrm{u}}$. The main question here is whether one can approximate the reduced evolution by a semigroup in the sense of (2.4); a natural guess is that it should be possible in case of a weak coupling. Since the reduced resolvent is of the form (2.3) we can express the corresponding measure, calculate the reduced propagator according to (2.2) and estimate the influence of the second term in (2.4). This leads to the following conclusion, essentially due to [De76]:

Theorem 3.2. *Under the stated assumptions there are positive C, g_0 such that*

$$\big| v(t) - A\, \mathrm{e}^{-iz_{\mathrm{p}}t} \big| < \frac{Cg^2}{t}$$

holds for all $t > 0$ and $|g| < g_0$ with $A := [1 - g^2 I'(z_{\mathrm{p}})]^{-1}$, where $I(z)$ is the integral appearing in the second one of the formulae (3.3).

The simple Friedrichs model described here has many extensions and in no way we intend to review and discuss them here limiting ourselves to a few brief remarks:

(a) Some generalization of the model cast it into a more abstract setting, cf. for example [Mo96, DR07, DJN11]. Others are more 'realistic' regarding it as a description of a system interacting with a field, either a caricature one-mode one [DE87-89] or considerably closer to physical reality [BFS98, HHH08] in a sense returning the model to its Lee version which stimulated interest to it.

(b) Friedrichs model clones typically use the simple procedure – attributed to Schur or Feshbach, and sometimes also to other people – we employed it to get relation (3.2) expressing projection of the resolvent to the subspace $\mathcal{H}_{\mathrm{u}}$; sometimes it is combined with a complex scaling.

(c) While most Friedrichs-type models concern perturbations of embedded eigenvalues some go further. As an example, let us mention a caricature model of a crystal interacting with a field [DEH04] in which the unperturbed Hamiltonian has a spectral band embedded in the continuous spectrum half-line referring to states of a lower band plus a field quantum. The perturbation turns the embedded band into a curve-shaped singularity in the lower complex half-plane with endpoints at the real axis. One can investigate in this framework decay of 'valence-band' states analogous to Theorem 3.2, etc.

(d) The weak-coupling behavior described in Theorem 3.2 can be viewed also from a different point of view, namely that the decay law converges to a fixed exponential function as $g \to 0$ when we pass to the rescaled time $t' = g^{-2}t$. This is usually referred to as *van Hove limit* in recognition of the paper [vH55]; the first rigorous treatment of the limit belongs to E.B. Davies, cf. [Da].

4. Resonances from perturbed symmetry

The previous section illustrates the most common mechanism of resonance emergence, namely perturbations of eigenvalues embedded in the continuum. A typical source of embedded eigenvalues is a symmetry of the system which prevents transitions from the corresponding localized state into a continuum one. Once such a symmetry is violated, resonances usually occur. Let us demonstrate that in a model describing a Schrödinger particle in a straight waveguide, perturbed by a potential or by a magnetic field, the idea of which belongs to J. Nöckel [Nö92].

4.1. Nöckel model

We consider two-dimensional 'electrons' moving in a channel with a potential well. The guide is supposed to be either a hard-wall strip $\Omega := \mathbb{R} \times S$ with $S = (-a, a)$, or alternatively the transverse confinement can be modelled by a potential in which case we have $S = \mathbb{R}$. The full Hamiltonian acting on $\mathcal{H} := L^2(\Omega)$ is given by

$$H(B, \lambda) := (-i\partial_x - By)^2 + V(x) - \partial_y^2 + W(y) + \lambda U(x, y)\,; \tag{4.1}$$

if Ω is a strip of width $2a$ the transverse potential W may be absent and we impose Dirichlet conditions at the boundary, $|y| = a$. The real-valued functions V describing the well in the waveguide – or a caricature quantum dot if you wish – and W are measurable, and the same is true for the potential perturbation U; further hypotheses will be given below. The number B is the intensity of the homogeneous magnetic field perpendicular to Ω to which the system is exposed.

The unperturbed Hamiltonian $H(0) := H(0,0)$ can be written in the form $h^V \otimes I + I \otimes h^W$ which means its spectrum is the 'sum' of the corresponding component spectra. If the spectrum of the transverse part h^W is discrete the embedded eigenvalues can naturally occur; we are going to see what happens with them under influence of the potential perturbation λU and/or the magnetic field. Let us first list the assumptions using the common notation $\langle x \rangle := \sqrt{1+x^2}$.

(a) $\lim_{|x|\to\infty} W(x) = +\infty$ holds if $S = \mathbb{R}$,

(b) $V \neq 0$ and $|V(x)| \leq \text{const}\, \langle x \rangle^{-2-\varepsilon}$ for some $\varepsilon > 0$, with $\int_{\mathbb{R}} V(x)\, \mathrm{d}x \leq 0$,

(c) the potential V extends to a function analytic in $\mathcal{M}_{\alpha_0} := \{z \in \mathbb{C} :\ |\arg z| \leq \alpha_0\}$ for some $\alpha_0 > 0$ and obeys there the bound of assumption (b),

(d) $|U(x,y)| \leq \text{const}\, \langle x \rangle^{-2-\varepsilon}$ holds for some $\varepsilon > 0$ and all $(x,y) \in \Omega$. In addition, it does not factorize, $U(x,y) \neq U_1(x) + U_2(y)$, and $U(\cdot, y)$ extends for each fixed $y \in S$ to an analytic function in $\mathcal{M}_{\alpha_0}$ satisfying there the same bound.

The assumption (a) ensures that the spectrum of $h^W := -\partial_y^2 + W(y)$, denoted as $\{\nu_j\}_{j=1}^{\infty}$, is discrete and simple, $\nu_{j+1} > \nu_j$. The same is true if $S = (-a, a)$ when we impose Dirichlet condition at $y = \pm a$, naturally except the case when W grows fast enough as $y \to \pm a$ to make the operator essentially self-adjoint. The assumption (b) says, in particular, that the local perturbation responsible for the occurrence of localized states is short-ranged and non-repulsive in the mean; it is well known that in this situation the longitudinal part $h^V := -\partial_x^2 + V(x)$ of the unperturbed Hamiltonian has a nonempty discrete spectrum,

$$\mu_1 < \mu_2 < \cdots < \mu_N < 0\,,$$

which is simple and finite [Si76, BGS77]; the corresponding normalized eigenfunctions ϕ_n, $n = 1, \ldots, N$, are exponentially decaying.

To be able to treat the resonances we need to adopt analyticity hypotheses stated in assumptions (c) and (d). Note that in addition to the matter of our interest the system can also have 'intrinsic' resonances associated with the operator h^V, however, the corresponding poles do not approach the real axis as the perturbation is switched off. In addition, they do not accumulate except possibly at the threshold [AC71], and if V decays exponentially even that is excluded [Je78, Lemma 3.4].

Since $\sigma_{\mathrm{c}}(h^V) = [0, \infty)$, the spectrum of the unperturbed Hamiltonian consists of the continuous part, $\sigma_{\mathrm{c}}(H(0)) = \sigma_{\mathrm{ess}}(H(0)) = [\nu_1, \infty)$, and the infinite family of eigenvalues

$$\sigma_{\mathrm{p}}(H(0)) = \{\, \mu_n + \nu_j :\ n = 1, \ldots, N\,,\ j = 1, 2, \ldots\}\,.$$

A finite number of them are isolated, while the remaining ones satisfying the condition $\mu_n+\nu_j > \nu_1$ are embedded in the continuum; let us suppose for simplicity that they coincide with none of the thresholds, $\mu_n+\nu_j \neq \nu_k$ for any k.

To analyze the resonance problem it is useful to employ the transverse-mode decomposition, in other words, to replace the original PDE problem by a matrix ODE one. Using the transverse eigenfunctions, $h^W\chi_j = \nu_j\chi_j$, we introduce the embeddings $\mathcal{J}_j$ and their adjoints acting as projections by

$$\begin{aligned} \mathcal{J}_j &: L^2(\mathbb{R}) \to L^2(\Omega), \qquad \mathcal{J}_j f = f\otimes\chi_j, \\ \mathcal{J}_j^* &: L^2(\Omega) \to L^2(\mathbb{R}), \qquad (\mathcal{J}_j^* g)(x) = (\chi_j, g(x,\cdot))_{L^2(S)}; \end{aligned}$$

then we replace $H(B,\lambda)$ by the matrix differential operator $\{H_{jk}(B,\lambda)\}_{j,k=1}^\infty$ with

$$\begin{aligned} H_{jk}(B,\lambda) &:= \mathcal{J}_j^* H(B,\lambda)\mathcal{J}_k = \left(-\partial_x^2 + V(x) + \nu_j\right)\delta_{jk} + \mathcal{U}_{jk}(B,\lambda), \\ \mathcal{U}_{jk}(B,\lambda) &:= 2iB\, m_{jk}^{(1)}\partial_x + B^2 m_{jk}^{(2)} + \lambda U_{jk}(x), \end{aligned}$$

where $m_{jk}^{(r)} := \int_S y^r \overline{\chi}_j(y)\chi_k(y)\,\mathrm{d}y$ and $U_{jk}(x) := \int_S U(x,y)\overline{\chi}_j(y)\chi_k(y)\,\mathrm{d}y$.

4.2. Resonances by complex scaling

Nöckel model gives us an opportunity to illustrate how the complex scaling method mentioned in the introduction can be used in a concrete situation. We apply here the scaling transformation to the longitudinal variable starting from the unitary operator

$$\mathcal{S}_\theta:\ (\mathcal{S}_\theta\psi)(x,y) = \mathrm{e}^{\theta/2}\psi(\mathrm{e}^\theta x, y), \quad \theta\in\mathbb{R},$$

and extending this map analytically to $\mathcal{M}_{\alpha_0}$ which is possible since the transformed Hamiltonians are of the form $H_\theta(B,\lambda) := \mathcal{S}_\theta H(B,\lambda)\mathcal{S}_\theta{}^{-1} = H_\theta(0)+\mathcal{U}_\theta(B,\lambda)$ with

$$H_\theta(0) := -\mathrm{e}^{-2\theta}\partial_x^2 - \partial_y^2 + V_\theta(x) + W(y), \tag{4.2}$$

where $V_\theta(x) := V(\mathrm{e}^{\theta x})$ and the interaction part

$$\mathcal{U}_\theta(B,\lambda) := 2i\,\mathrm{e}^{-\theta}By\,\partial_x + B^2y^2 + \lambda U_\theta(x,y)$$

with $U_\theta(x,y) := U(\mathrm{e}^{\theta x}, y)$. Thus in view of the assumptions (c) and (d) they constitute a type (A) analytic family of m-sectorial operators in the sense of [Ka] for $|\mathrm{Im}\,\theta| < \min\{\alpha_0, \pi/4\}$. Denoting $R_\theta(z) := (H_\theta(0)-z)^{-1}$ one can check [DEM01] that

$$\|\mathcal{U}_\theta(B,\lambda)R_\theta(\nu_1+\mu_1-1)\| \le c(|B|+|B|^2+|\lambda|) \tag{4.3}$$

holds for $|\mathrm{Im}\,\theta| < \min\{\alpha_0,\pi/4\}$, and consequently, the operators $H_\theta(B,\lambda)$ also form a type (A) analytic family for B and λ small enough. The free part (4.2) of the transformed operator separates variables, hence its spectrum is

$$\sigma\left(H_\theta(0)\right) = \bigcup_{j=1}^{\infty}\left\{\,\nu_j + \sigma\left(h_\theta^V\right)\right\}, \tag{4.4}$$

where $h_\theta^V := -\mathrm{e}^{-2\theta}\partial_x^2 + V_\theta(x)$. Since the potential is dilation-analytic by assumption, we have a typical picture: the essential spectrum is rotated into the lower half-plane revealing (fully or partly) the discrete spectrum of the non-selfadjoint operator h_θ^V which is independent of θ; we have

$$\sigma\left(h_\theta^V\right) = \mathrm{e}^{-2\theta}\mathbb{R}^+ \cup \{\mu_1,\dots,\mu_N\} \cup \{\rho_1,\rho_2,\dots\}\,, \tag{4.5}$$

where ρ_r are the 'intrinsic' resonances of h^V. In view of the assumptions (c) and $\mu_n+\nu_j \neq \nu_k$ for no k, the supremum of $\operatorname{Im}\rho_k$ over any finite region of the complex plane which does not contain any of the points ν_k is negative, hence each eigenvalue $\mu_n+\nu_j$ has a neighbourhood containing none of the points $\rho_k+\nu_{j'}$. Consequently, the eigenvalues of $H_\theta(0)$ become isolated once $\operatorname{Im}\theta > 0$. Using the relative boundedness (4.3) we can draw a contour around an unperturbed eigenvalue and apply perturbation theory; for simplicity we shall consider only the non-degenerate case when $\mu_n+\nu_j \neq \mu_{n'}+\nu_{j'}$ for different pairs of indices.

We fix an unperturbed eigenvalue $e_0 = \mu_n+\nu_j$ and choose $\theta = i\beta$ with a $\beta>0$; then in view of (4.4) and (4.5) we may chose a contour Γ in the resolvent set of $H_\theta(0)$ which encircles just the eigenvalue e_0. We use the symbol P_θ for the eigenprojection of $H_\theta(0)$ referring to e_0 and set

$$S_\theta^{(p)} := \frac{1}{2\pi i}\int_\Gamma \frac{R_\theta(z)}{(e_0-z)^p}\,\mathrm{d}z$$

for $p=0,1,\dots$, in particular, $S_\theta^{(0)} = -P_\theta$ and $\hat{R}_\theta(z) := S_\theta^{(1)}$ is the reduced resolvent of $H_\theta(0)$ at the point z. The bound (4.3) implies easily

$$\left\|\mathcal{U}_\theta(B,\lambda)S_\theta^{(p)}\right\| \le c\,\frac{|\Gamma|}{2\pi}\left(\mathrm{dist}(\Gamma,e_0)\right)^{-p}(|B|+|B|^2+|\lambda|)$$

with some constant c for all $\operatorname{Im}\theta \in (0,\alpha_0)$ and $p\ge 0$. It allows us to write the perturbation expansion. Since $e_0=\mu_n+\nu_j$ holds by assumption for a unique pair of the indices, we obtain using [Ka, Sec. II.2] the following convergent series

$$e(B,\lambda) = \mu_n+\nu_j+\sum_{m=1}^{\infty} e_m(B,\lambda)\,, \tag{4.6}$$

where $e_m(B,\lambda) = \sum_{p_1+\dots+p_m=m-1}\frac{(-1)^m}{m}\operatorname{Tr}\prod_{i=1}^m \mathcal{U}_\theta(B,\lambda)S_\theta^{(p_i)}$. Using the above estimate we can estimate the order of each term with respect to the parameters. We find $e_m(B,\lambda) = \sum_{l=0}^m \mathcal{O}\left(B^l\lambda^{m-l}\right)$, in particular, we have $e_m(B)=\mathcal{O}(B^m)$, and $e_m(\lambda)=\mathcal{O}(\lambda^m)$ for pure magnetic and pure potential perturbations, respectively.

The lowest-order terms in the expansion (4.6) can be computed explicitly. In the non-degenerate case, $\dim P_\theta = 1$, we have $e_1^{j,n}(B,\lambda) = \operatorname{Tr}\left(\mathcal{U}_\theta(B,\lambda)P_\theta\right)$. After a short calculation we can rewrite the expression at the right-hand side in the form $2iBm_{jj}^{(1)}(\phi_n,\phi_n') + B^2m_{jj}^{(2)} + \lambda\,(\phi_n,U_{jj}\phi_n)$. Moreover, $i\,(\phi_n,\phi_n') = (\phi_n, i\partial_x\phi_n)$ is (up to a sign) the group velocity of the wavepacket, which is zero in a stationary state; recall that eigenfunction ϕ_n of h^V is real valued up to a phase factor. In other words,

$$e_1^{j,n}(B,\lambda) = B^2\int_S y^2\,|\chi_j(y)|^2\,\mathrm{d}y + \lambda\int_{\mathbb{R}\times S} U(x,y)\,|\phi_n(x)\chi_j(y)|^2\,\mathrm{d}x\,\mathrm{d}y \tag{4.7}$$

with the magnetic part independent of n. As usual in such situations the first-order correction is real valued and thus does not contribute to the resonance width.

The second term in the expansion (4.6) can be computed in the standard way [RS, Sec.XII.6]; taking the limit $\mathrm{Im}\,\theta \to 0$ in the obtained expression we get

$$e_2^{j,n}(B,\lambda) = -\sum_{k=1}^{\infty} \Big(\mathcal{U}_{jk}(B,\lambda)\phi_n, \Big(\big(h^V - e_0 + \nu_k - i0\big)^{-1} \Big)\hat{} \; \mathcal{U}_{jk}(B,\lambda)\phi_n \Big) \,. \qquad (4.8)$$

We shall calculate the imaginary part which determines the resonance width in the leading order. First we note that it can be in fact expressed as a finite sum. Indeed, $k_{e_0} := \max\{k :\, e_0 - \nu_k > 0\}$ is finite and nonzero if the eigenvalue e_0 is embedded, otherwise we set it equal to zero. It is obvious that $\mathcal{R}_k := \big(\big(h^V - e_0 + \nu_k - i0\big)^{-1} \big)\hat{}$ is Hermitian for $k > k_{e_0}$, hence the corresponding terms in (4.8) are real and

$$\mathrm{Im}\, e_2^{j,n}(B,\lambda) = \sum_{k=1}^{k_{e_0}} (\mathcal{U}_{jk}(B,\lambda)\phi_n, (\mathrm{Im}\,\mathcal{R}_k)\mathcal{U}_{jk}(B,\lambda)\phi_n) \,.$$

The operators $\mathrm{Im}\,\mathcal{R}_k$ can be expressed by a straightforward computation [DEM01]. To write the result we need $\omega(z) := \big[I + |V|^{1/2}(-\partial_x^2 - z)^{-1}|V|^{1/2}\mathrm{sgn}\,(V) \big]^{-1}$, in other words, the inverse to the operator acting as

$$\big(\omega^{-1}(z)f\big)(x) = f(x) + \frac{i|V(x)|^{1/2}}{2\sqrt{z}} \int_{\mathbb{R}} \mathrm{e}^{i\sqrt{z}|x-x'|} |V(x')|^{1/2} \mathrm{sgn}\, V(x')\, f(x')\, \mathrm{d}x' \,.$$

We also need the trace operator $\tau_E^\sigma :\, \mathcal{H}^1 \to \mathbb{C}$ which acts on the first Sobolev space $W^{1,2}$ as $\tau_E^\sigma \phi := \hat{\phi}(\sigma\sqrt{E})$ for $\sigma = \pm$ and $E > 0$ where $\hat{\phi}$ is the Fourier transform of ϕ. Armed with these notions we can write the imaginary part of the resonance pole position up to higher-order terms as

$$\begin{aligned} \mathrm{Im}\, e_2^{j,n}(B,\lambda) &= \sum_{k=1}^{k_{e_0}} \sum_{\sigma=\pm} \frac{\pi}{2\sqrt{e_0 - \nu_k}} \big| \tau^\sigma_{e_0-\nu_k} \omega(e_0 - \nu_k + i0)\, \mathcal{U}_{jk}(B,\lambda)\phi_n \big|^2 \qquad (4.9) \\ &= \sum_{k=1}^{k_{e_0}} \sum_{\sigma=\pm} \frac{\pi}{\sqrt{e_0 - \nu_k}} \Big\{ -2B^2\, |m_{jk}^{(1)}|^2\, \big| \tau^\sigma_{e_0-\nu_k} \omega(e_0 - \nu_k + i0)\phi_n' \big|^2 \\ &\quad + 2\lambda B\, m_{jk}^{(1)}\, \mathrm{Im}\, \Big(\tau^\sigma_{e_0-\nu_k} \omega(e_0 - \nu_k + i0)\phi_n' \,, \tau^\sigma_{e_0-\nu_k} \omega(e_0 - \nu_k + i0) U_{jk}\phi_n \Big) \\ &\quad - \frac{\lambda^2}{2} \big| \tau^\sigma_{e_0-\nu_k} \omega(e_0 - \nu_k + i0)\, U_{jk}\phi_n \big|^2 \Big\} + \mathcal{O}(B^3) + \mathcal{O}(B^2\lambda) \,, \end{aligned}$$

where as usual $f(E + i0) = \lim_{\varepsilon\to 0+} f(E + i\varepsilon)$. Let us summarize the results:

Theorem 4.1. *Assume* (a)–(d) *and suppose that an unperturbed eigenvalue* $e_0 = \mu_n + \nu_j > \nu_1$ *is simple and coincides with no threshold* ν_k*. For small enough* B *and* λ *the Nöckel model Hamiltonian* (4.1) *has a simple resonance pole the position of which is given by the relations* (4.6)*–*(4.8)*. The leading order in the expansion obtained by neglecting the error terms in* (4.9) *is the Fermi golden rule in this case.*

The symmetry in this example is somewhat hidden; it consists of the factorized form of the unperturbed Hamiltonian $H(0)$ which makes it reducible by projections to subspaces associated with the transverse modes. It is obvious that both the potential perturbation – recall that we assumed $U(x,y) \neq U_1(x)+U_2(y)$ – and the magnetic field destroy this symmetry turning thus embedded eigenvalues coming from higher transverse modes into resonances. At the same time, the described decomposition may include other, more obvious symmetries. For instance, if the potential W is even with respect to the strip axis – including the case when $S=(-a,a)$ and $W=0$ – the unperturbed Hamiltonian commutes with the transverse parity operator, $\psi(x,y) \mapsto \psi(x,-y)$, and the transversally odd states are orthogonal to the even ones so embedded eigenvalues arise.

Nöckel model is by far not the only example of this type. We limit ourselves here to quoting one more. Consider an *acoustic waveguide* in the form of a planar strip of width $2a$ into which we place an axially symmetric obstacle; the corresponding Hamiltonian acts as Laplacian with Neumann condition at the boundary, both of the strip and the obstacle. Due to the axial symmetry the odd part of the operator gives rise to at least one eigenvalue in the interval $\big(0, \frac{1}{4}(\frac{\pi}{a})^2\big)$ which is embedded into the continuous spectrum covering the whole positive real axis [ELV94]. If the obstacle is shifted by ε in the direction perpendicular to the axis, such an eigenvalue turns again into a resonance for the position of which one can derive an expansion in powers of ε analogous to Theorem 4.1, cf. [APV00].

5. Point contacts

The resonance models discussed in the previous two sections show that we should be more precise speaking about *solvable* models. The question naturally is what we have finally to *solve* when trying to get conclusions such as formulae for resonance pole positions. In both cases we have been able to derive weak-coupling expansions with explicit leading terms which could be regarded as confirmation of the Fermi golden rule for the particular model. One has to look, however, into which sort of problem the search for resonances was turned. For the Friedrichs model it was the functional equation $w(z,g)=z$ with the left-hand side given by (3.3), and a similar claim is true for its clones, while in the Nöckel model case we had to perform spectral analysis of the non-selfadjoint operator[1] $H_\theta(B,\lambda)$.

Not only the latter has been more difficult in the above discussion, the difference becomes even more apparent if we try to go beyond the weak-coupling approximation. Following the pole trajectory over a large interval of coupling parameters may not be easy even if its position is determined by a functional equation and one have to resort usually to numerical methods, however, it is still much easier than to analyze a modification of the original spectral problem. Recall that for the Friedrichs model pole trajectories were investigated already in [Hö58] where

[1]The same is true also for most ‘realistic’ descriptions of resonances using complex scaling, in particular, in the area of atomic and molecular physics – see, e.g., [RS, Sec. XII.6] or [Mo98].

it had been shown, in particular, that for strong enough coupling the pole may return to the (negative part of the) real axis becoming again a bound state.

In the rest of this review we will deal with models which are 'solvable' at least in the sense of the Friedrichs model, that is, their resonances are found as roots of a functional – sometimes even algebraic – equation. In this section we will give examples showing that this is often the case in situations where the interaction responsible for occurrence of the resonances is of point or contact type.

5.1. A simple two-channel model

The first model to consider here will describe a system the state space of which has two subspaces corresponding to two internal states; the coupling between them is of a *contact nature*. To be specific, one can think of a system consisting of a neutron and a nucleus having just two states, the ground state and an excited one. Their relative motion can be described in the Hilbert space $L^2(\mathbb{R}^3) \oplus L^2(\mathbb{R}^3)$; we suppose that the reduced masses is the two channels are the same and equal to $\frac{1}{2}$ so that the Hamiltonian acts on functions supported away from the origin of the coordinates as $-\Delta$ and $-\Delta + E$, respectively, where $E > 0$ is the energy difference between the ground and the excited states.

Before proceeding further, let us note that the above physical interpretation of the model coming from [Ex91] is not the only possible. The two channels can be alternatively associated, for instance, with two spin states; this version of the model was worked out in [CCF09], also in dimensions one and two.

To construct the Hamiltonian we start from the direct sum $A_0 = A_{0,1} \oplus A_{0,2}$ where the component operators act as $A_{0,1} := -\Delta$ and $A_{0,2} := -\Delta + E$, respectively, being defined on $W^{2,2}(\mathbb{R}^3 \setminus \{0\})$. It is not difficult to check that A_0 is a symmetric operator with deficiency indices $(2,2)$; we will choose the model Hamiltonian among its self-adjoint extensions. The analysis can be simplified using the rotational symmetry, since the components of A_0 referring to nonzero values of the angular momentum are essentially self-adjoint, and therefore a nontrivial coupling is possible in the s-wave only. As usual we pass to reduced radial wave functions $f:\, f(r) := r\psi(r)$; we take $\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2$ with $\mathcal{H}_j := L^2(\mathbb{R}^+)$ as the state space of the problem. The construction starts from the operator $H_0 = H_{0,1} \oplus H_{0,2}$, where

$$H_{0,1} := -\frac{\mathrm{d}^2}{\mathrm{d}r^2}\,, \quad H_{0,2} := -\frac{\mathrm{d}^2}{\mathrm{d}r^2} + E\,, \quad D(H_{0,j}) = W_0^{2,2}(\mathbb{R}^+)\,,$$

which has again deficiency indices $(2,2)$ and thus a four-parameter family of self-adjoint extensions. They can be characterized by means of boundary conditions: for each matrix $\mathcal{A} = \begin{pmatrix} a & c \\ \bar{c} & b \end{pmatrix}$ with $a, b \in \mathbb{R}$ and $c \in \mathbb{C}$ we denote by $H_{\mathcal{A}}$ the operator given by the same differential expression as H_0 with the domain $D(H_{\mathcal{A}}) \subset D(H_0^*) = W^{2,2}(\mathbb{R}^+) \oplus W^{2,2}(\mathbb{R}^+)$ specified by the conditions

$$f_1'(0) = af_1(0) + cf_2(0)\,, \qquad f_2'(0) = \bar{c}f_1(0) + bf_2(0)\,; \tag{5.1}$$

it is easy to check that any such $H_{\mathcal{A}}$ is a self-adjoint extension of H_0. There may be other extensions, say, with decoupled channels corresponding to $a = \infty$ or $b = \infty$ but it is enough for us to consider 'most part' of them given by (5.1).

If the matrix $\mathcal{A}$ is real the operator $H_{\mathcal{A}}$ is invariant with respect to time reversal. The channels are not coupled if $c = 0$; in that case $H_{\mathcal{A}} = H_a \oplus H_b$ where the two operators correspond to the s-wave parts of the point-interaction Hamiltonians $H_{\alpha,0}$ and $H_{\beta,0}$ in the two channels [AGHH] with the interaction strengths $\alpha := \frac{a}{4\pi}$ and $\beta := \frac{b}{4\pi}$, respectively, and its spectrum is easily found. To determine $\sigma(H_{\mathcal{A}})$ in the coupled case, we have to know its resolvent which can be determined by means of Krein's formula using the integral kernel $G_{\mathrm{D}}(r,r';k) = \mathrm{diag}\big(\frac{\mathrm{e}^{ik|r+r'|}-\mathrm{e}^{ik|r-r'|}}{2ik}, \frac{\mathrm{e}^{i\kappa|r+r'|}-\mathrm{e}^{i\kappa|r-r'|}}{2i\kappa}\big)$, where $\kappa := \sqrt{k^2-E}$, of the operator H_{D} with Dirichlet decoupled channels. The kernel of $(H_{\mathcal{A}}-z)^{-1}$ for $z \in \rho(H_{\mathcal{A}})$ equals

$$G_{\mathcal{A}}(r,r';k) = G_{\mathrm{D}}(r,r';k) + D(k)^{-1} \begin{pmatrix} (b-i\kappa)\,\mathrm{e}^{ik(r+r')} & -\,c\,\mathrm{e}^{(ikr+\kappa r')} \\ -\,\bar{c}\,\mathrm{e}^{i(\kappa r+kr')} & (a-ik)\,\mathrm{e}^{i\kappa(r+r')} \end{pmatrix},$$

where as usual $k := \sqrt{z}$ and $D(k) := (a-ik)(b-i\kappa) - |c|^2$.

It is straightforward to check that pole singularities of the above the resolvent can come only from zeros of the 'discriminant' $D(k)$. In the decoupled case, i.e., if $c = 0$ and $\mathcal{A}_0 = \binom{a\ 0}{0\ b}$, the expression factorizes, and consequently, it vanishes *iff* $k = -ia$ or $\kappa = -ib$. Several different situations may arise:

- If $a < 0$ the operator $H_{\mathcal{A}_0}$ has eigenvalue $-a^2$ corresponding to the eigenfunction $f(r) = \sqrt{-2a}\,\binom{\mathrm{e}^{ar}}{0}$ while for $a \geq 0$ the pole now corresponds to a zero-energy resonance or an antibound state
- If $b < 0$, then $H_{\mathcal{A}_0}$ has eigenvalue $E-b^2$ corresponding to $f(r) = \sqrt{-2b}\,\binom{0}{\mathrm{e}^{br}}$, otherwise it has a zero-energy resonance or an antibound state.

The continuous spectrum of the decoupled operator covers the positive real axis being simple in $[0, E)$ and of multiplicity two in $[E, \infty)$. We are interested mainly in the case when both a, b are negative and $b^2 < E$; under the last condition the eigenvalue of H_b is embedded in the continuous spectrum of H_a.

Let us next turn to the interacting case, $c \neq 0$. Since the deficiency indices of H_0 are finite, the essential spectrum is not affected by the coupling. To find the eigenvalues and/or resonances of $H_{\mathcal{A}}$, we have to solve the equation

$$(a-ik)\left(b-i\sqrt{k^2-E}\right) = |c|^2. \tag{5.2}$$

It reduces to a quartic equation, and can therefore be solved in terms of radicals; for simplicity we limit ourselves to the *weak-coupling case* when one can make the following conclusion [Ex91].

Theorem 5.1.

(a) *Let $\sigma_{\mathrm{p}}\big(H_{\mathcal{A}_0}\big)$ be simple, $-a^2 \neq E-b^2$, then the perturbed first-channel bound/antibound state behaves for small $|c|$ as*

$$e_1(c) = -a^2 + \frac{2a|c|^2}{b+\sqrt{a^2+E}} + \frac{a^2-E-b\sqrt{a^2+E}}{\sqrt{a^2+E}\,\big(b+\sqrt{a^2+E}\big)^3}|c|^4 + \mathcal{O}(|c|^6)\,.$$

In particular, zero-energy resonance corresponding to $a = 0$ turns into an antibound state if $H_{\mathcal{A}_0}$ has an isolated eigenvalue in the second channel, $b < -\sqrt{E}$, and into a bound state otherwise.

(b) *Under the same simplicity assumption, if $H_{\mathcal{A}_0}$ has isolated eigenvalue in the second channel, $b < -\sqrt{E}$, the perturbation shifts it as follows*

$$e_2(c) = E - b^2 + \frac{2b|c|^2}{a+\sqrt{b^2-E}} + \frac{b^2+E-a\sqrt{b^2-E}}{\sqrt{b^2-E}\left(a+\sqrt{b^2-E}\right)^3}\,|c|^4 + \mathcal{O}(|c|^6)\,.$$

On the other hand, if $H_{\mathcal{A}_0}$ has embedded eigenvalue, $-\sqrt{E} < b < 0$, it turns under the perturbation into a pole of the analytically continued resolvent with

$$\begin{aligned}\operatorname{Re} e_2(c) &= E - b^2 + \frac{2ab|c|^2}{a^2-b^2+E} + \mathcal{O}(|c|^4)\,,\\ \operatorname{Im} e_2(c) &= \frac{2b|c|^2\sqrt{E-b^2}}{a^2-b^2+E} + \mathcal{O}(|c|^4)\,.\end{aligned}$$

(c) *Finally, let $H_{\mathcal{A}_0}$ have an isolated eigenvalue of multiplicity two, $b=-\sqrt{a^2+E}$,; then under the perturbation it splits into*

$$e_{1,2}(c) = -a^2 \mp 2\sqrt{-a}\,\sqrt[4]{a^2+E}\,|c| + \frac{2a^4+4a^2E+E^2}{2a(a^2+E)^{3/2}}\,|c|^2 + \mathcal{O}(|c|^3)\,.$$

The model can be investigated also from the scattering point of view. Since the couplings is a rank-two perturbation of the free resolvent, the existence and completeness of the wave operators $\Omega_\pm(H_{\mathcal{A}}, H_{\mathcal{A}_0})$ follow from Birman–Kuroda theorem [RS, Sec. XI.3]. It is also easy to check that the scattering is asymptotically complete, what is more interesting is the explicit form of the S-matrix. To find it we look for generalized eigenfunctions of the form $f(r) = \left(e^{-ikr} - A\mathrm{e}^{ikr}, B\mathrm{e}^{i\kappa r}\right)^{\mathrm{T}}$ which belong *locally* to the domain of $H_{\mathcal{A}}$. Using boundary conditions (5.1) we find

$$A = S_0(k) = \frac{(a+ik)(b-i\kappa) - |c|^2}{D(k)}\,, \qquad B = \frac{2ik\bar{c}}{D(k)}\,.$$

If the second channel is closed, $k^2 \le E$, the scattering is elastic, $|A| = 1$. We are interested primarily in the case when $H_{\mathcal{A}_0}$ has an embedded eigenvalue which turns under the perturbation into a resonant state whose lifetime is

$$T(c) := -\frac{a^2-b^2+E}{4b|c|^2\sqrt{E-b^2}}\,\left(1+\mathcal{O}(|c|^2)\right)\,;$$

inspecting the phase shift we see that it has a jump by π in the interval of width of order $2\operatorname{Im} e_2(c)$ around $\operatorname{Re} e_2(c)$. More specifically, writing the on-shell S-matrix conventionally through the phase shift as $S_0(k) = e^{2i\delta_0(k)}$ we have

$$\delta_0(k) = \arctan\frac{k(b+\sqrt{E-k^2})}{a(b+\sqrt{E-k^2}) - |c|^2} \pmod{\pi}\,.$$

The resonance is then seen as a local change of the transmission probability (and related quantities such as the scattering cross section), the sharper it is the closer the pole is to the real axis. This is probably the most common way in which resonances are manifested, employed in papers too numerous to be quoted here.

On the other hand, if the second channel is open, $k^2 > E$, the reflection and transmission amplitudes given above satisfy $|A|^2 + \frac{\kappa}{k}|B|^2 = 1$. The elastic scattering is now non-unitary since $B \neq 0$ which means that the 'nucleus' may now leave the interaction region in the excited state. The said relation between the amplitudes can alternatively be written as $|S_{0,1\to 1}(k)|^2 + |S_{0,1\to 2}(k)|^2 = 1$ which is a part of the full two-channel S-matrix unitarity condition.

The model also allows us to follow the time evolution of the resonant state, in particular, to analyze the pole approximation (2.4) in this particular case. The natural choice for the 'compound nucleus' wave function is the eigenstate of the unperturbed Hamiltonian,

$$f \,:\, f(r) = \sqrt{-2b}\begin{pmatrix} 0 \\ \mathrm{e}^{br} \end{pmatrix}. \tag{5.3}$$

Using the explicit expression of the resolvent we find

$$(f, (H_{\mathcal{A}} - k^2)^{-1} f) = \frac{|c|^2 + (a-ik)(b+i\kappa)}{(b+i\kappa)^2\big[|c|^2 - (a-ik)(b-i\kappa)\big]}\,.$$

The reduced evolution is given by (2.2); using the last formula, evaluating the integral by means of the residue theorem and estimating the remainder we arrive after a straightforward computation to the following conclusion [Ex91].

Theorem 5.2. *Assume $a \neq 0$ and $-\sqrt{E} < b < 0$. The reduced propagator of the resonant state* (5.3) *is given by*

$$v_{\mathcal{A}}(t) = \Bigg\{ \mathrm{e}^{-ik_2^2 t} - |c|^2 \Bigg[\frac{2(|a|-a)b}{(a^2-b^2+E)^2}\,\mathrm{e}^{-ik_1^2 t} + \frac{ib}{\sqrt{E-b^2}(a-i\sqrt{E-b^2})^2}\,\mathrm{e}^{-ik_2^2 t} + \frac{4b}{\pi}\,\mathrm{e}^{-\pi i/4}\int_0^\infty \frac{z^2 \mathrm{e}^{-z^2 t}\,\mathrm{d}z}{(z^2+ia^2)(z^2-i(E-b^2))^2} \Bigg] \Bigg\} \big(1 + \mathcal{O}(|c|^2)\big)$$

and the decay law is

$$P_{\mathcal{A}}(t) = \Bigg\{ \mathrm{e}^{2(\mathrm{Im}\, e_2)t} - 2|c|^2 \mathrm{Re}\Bigg[\frac{2(|a|-a)b}{(a^2-b^2+E)^2}\,\mathrm{e}^{-i(k_1^2-\bar{k}_2^2)t} + \frac{ib}{\sqrt{E-b^2}(a-i\sqrt{E-b^2})^2}\,e^{2(\mathrm{Im}\, e_2)t} + \frac{4b}{\pi}\,e^{i(\bar{k}_2^2 t-\pi/4)}\int_0^\infty \frac{z^2 e^{-z^2 t}\,\mathrm{d}z}{(z^2+ia^2)(z^2-i(E-b^2))^2} \Bigg] \Bigg\} \big(1 + \mathcal{O}(|c|^2)\big)\,,$$

where $e_j = e_j(c) =: k_j^2$, $j = 1, 2$, are specified in Theorem 5.1.

Hence we have an explicit formula for deviations from the exponential decay law. Some of its properties, however, may not be fully obvious. For instance, the initial decay rate vanishes, $\dot{P}_{\mathcal{A}}(0+) = 0$, since $\mathrm{Im}\,(f,(H_{\mathcal{A}}-\lambda)^{-1}f) = \mathcal{O}(\lambda^{-5/2})$ as $\lambda \to \infty$, cf. Proposition 6.1 below. On the other hand, the long-time behavior depends substantially on the spectrum of the unperturbed Hamiltonian. If $H_{\mathcal{A}_0}$ has an eigenvalue in the first channel, then the decay law contains a term of order of $|c|^4$, which does not vanish as $t \to \infty$; it comes from the component of the first-channel bound state contained in the resonant state (5.3).

The last name fact it is useful to keep in mind when we speak about an unstable state *lifetime*. It is a common habit, motivated by the approximation (2.4), to identify the latter with the inverse distance of the pole from the real axis as we did above when writing $T(c)$. If the decay law is differentiable, however, $-\dot{P}_{\mathcal{A}}(t)$ expresses the probability density of decay at the instant t and a simple integration by parts allows us to express the average time for which the initial state survives as $T_{\mathcal{A}} = \int_0^\infty P_{\mathcal{A}}(t)\,\mathrm{d}t$; this quantity naturally diverges if $\lim_{t\to\infty} P_{\mathcal{A}}(t) \neq 0$.

5.2. K-shell capture model: comparison to stochastic mechanics

The above model has many modifications, we will describe briefly two of them. The first describes a β-decay process in which an atomic electron is absorbed by the nucleus and decays through the reaction $e{+}p \to n{+}\nu$ with a neutrino emitted. One usually speaks about a *K-shell capture* because the electron comes most often from the lowest energy orbital, however, from the theoretical point any orbital mode can be considered. We assume again spherical symmetry and take $\mathcal{H} = \mathcal{H}_1 \oplus \mathcal{H}_2$ with $\mathcal{H}_j := L^2(\mathbb{R}^+)$ as the state space. The first component refers to the (s-wave part of) atomic wave function, the other is a caricature description of the decayed states; we neglect the fact that neutrino is a relativistic particle.

The departing point of the construction is again a non-selfadjoint operator of the form $H_0 = H_{0,1} \oplus H_{0,2}$, the components of which act as

$$H_{0,1} := -\frac{1}{2m}\frac{\mathrm{d}^2}{\mathrm{d}r^2} + V_\ell(r)\,, \quad H_{0,2} := -\frac{1}{2M}\frac{\mathrm{d}^2}{\mathrm{d}x^2} - E \tag{5.4}$$

with the domains $D(H_{0,1}) = \{f \in W^{2,2}(\mathbb{R}^+) :\ u(R_j-) = u(R_j+) = 0\}$ for fixed $0 < R_1 < R_2 < \cdots < R_N$ – we add the requirement $f(0+) = 0$ if the angular momentum $\ell = 0$ – and $D(H_{0,2}) = \{W^{2,2}(\mathbb{R}^+) :\ f(0+) = f'(0+) = 0\}$. Here as usual $V_\ell(r) = V(r) + \frac{\ell(\ell+1)}{2mr^2}$ and the potential is supposed to satisfy the conditions

$$\lim_{r\to\infty} V(r) = 0\,, \quad \limsup_{r\to 0}\, rV(r) = \gamma < \infty\,,$$

under which the operator H_0 is symmetric with deficiency indices $(N+1, N+1)$. Of all its self-adjoint extensions we choose a subclass that (i) allows us to switch off the coupling and (ii) couples each sphere *locally* to the other space. The adjoint operator H_0^* acts again as (5.4); the extensions $H(a)$ described by $a = (a_1, \ldots, a_N)$

are specified by the boundary conditions

$$u'(R_j+) - u'(R_j-) = a_j f'(0+)\,, \quad j = 1,\dots,N \;\text{ and } \sum_{j=1}^{N} \bar{a}_j u(R_j) = -\frac{m}{M}\, f(0+)\,;$$

it is easy to see that under them the appropriate boundary form vanishes, the channels are decoupled for $a = 0$, and the Hamiltonians H_a are time-reversal invariant.

To solve the resonance problem in the model we have to find the resolvent of $H(a)$ which can be again done using Krein's formula. We will describe the resolvent projection to the 'atomic' channel referring for the full expression and the proof to [ET92]. We introduce the kernel

$$G_1(r,s;k^2) = \frac{1}{W(v_k,u_k)}\, u_k(r_<)v_k(r_>)\,,$$

where as usual $r_< := \min\{r,s\}$, $r_> := \max\{r,s\}$, and the functions u_k, v_k are solutions to $-\frac{1}{2m}\,u'' + Vu = \frac{k^2}{2m}\,u$ such that $u_k(0+) = 0$ and v_k is L^2 around ∞, and furthermore, $W(v_k,u_k) := v_k(r)u_k'(r) - v_k'(r)u_k(r)$ is their Wronskian.

Before stating the result, let us mention that the model can also cover the situation when the electron can be absorbed anywhere within the volume of the nucleus approximating this behavior by a family of equidistant spheres with $R_j := jR/N$, $j = 1,\dots,N$, where R is the nucleon radius. Let $a : [0,R] \to \mathbb{R}$ be a bounded piecewise continuous function understood as 'decay density', and take $H(a^N)$ corresponding to $a_j^N := \frac{R}{N}\, a\big(\frac{jR}{N}\big)$. On a formal level, the limit $N \to \infty$ leads to an operator describing the two channels coupled through the boundary conditions

$$u''(r) = a(r)f'(0+)\,, \qquad \int_0^R a(s)u(s)\,\mathrm{d}s = -\frac{m}{M}\, f(0+)\,,$$

however, we limit ourselves to checking the strong resolvent convergence [ET92].

Theorem 5.3. *The projection of the resolvent $(H(a)-z)^{-1}$ to the 'atomic' channel is an integral operator with the kernel*

$$G_1(r,s;z) + \sum_{j,k=1}^{N} \frac{i\kappa M a_j \bar{a}_k G_1(r,R_j;z) G_1(R_k,s;z)}{m - i\kappa M \sum_{i,l=1}^{N} a_i \bar{a}_l G_1(R_l,R_i;z)}\,.$$

The projections of $(H(a^N)-z)^{-1}$ converge as $N \to \infty$ to operator with the kernel

$$G_1(r,s;z) + \frac{i\kappa M \phi_k(r)\phi_k(s)}{m - i\kappa M \int_0^R \int_0^R a(r)a(s)G_1(r,s;z)\,\mathrm{d}r\mathrm{d}s}\,,$$

where $\phi_k := \int_0^R a(s)G_1(\cdot,s;z)\,\mathrm{d}s$, in the strong resolvent sense.

The singularities correspond to zeros of the denominators in the above expression. As an example, consider the 'atom' with Coulomb potential,

$$V_\ell(r) = \frac{\gamma}{r} + \frac{\ell(\ell+1)}{2mr^2}\,, \quad \gamma < 0\,,$$

which has in the decoupled case, $a = 0$, poles at $k_n = -\frac{im\gamma}{n}$, $n = 1, 2, \dots$. The Green function G_1 can be expressed in terms of the standard Coulomb wave functions $\psi_{n\ell m}(r,\vartheta,\varphi) = R_{n\ell}(r)Y_{\ell m}(\vartheta,\varphi)$. To analyze weak-coupling behavior of the poles, we restrict ourselves to two cases, a *surface-supported decay* when $N = 1$ and a *volume-supported decay* with a constant 'density' when $a(r) = a$ is a constant function on $[0, R]$. We put $\kappa_n := \sqrt{2mE - \left(\frac{m\gamma}{n}\right)^2}$ and introduce the form factor

$$B_n(r) := \begin{cases} R\,R_{n\ell}(r) & \dots \quad \text{surface-supported decay} \\ \int_0^R r\,R_{n\ell}(r)\,\mathrm{d}r & \dots \quad \text{volume-supported decay} \end{cases}$$

A straightforward calculation [ET92] then yields the shifted pole positions,

$$\frac{k_n^2(a)}{2m} = -\frac{m\gamma^2}{2n} - \frac{i}{4}\,a^2 m\kappa_n\gamma^3(2\ell+1)!\,B_n(R)^2 + \mathcal{O}(a^4)\,.$$

We are interested particularly in the situation where the unperturbed eigenvalue is embedded, $n > \sqrt{\frac{m\gamma^2}{2E}}$, when κ_n is real and the coupling shifts the pole into the lower complex half-plane giving rise to the resonant state with the lifetime

$$T_n(a) = \frac{8a^2(B_n(R))^{-2}}{m\kappa_n\gamma^3(2\ell+1)!} + \mathcal{O}(a^0)\,.$$

In the case of the real decay, of course, all the unperturbed eigenvalues are embedded and the K-shell contribution is dominating. It has the shortest lifetime since $R_{n\ell}(0)$ is nonzero for $\ell = 0$ only and $m\gamma R \ll 1$, typically of order 10^{-4}, so the form factor value is essentially determined by the wave function value at the origin.

The K-shell capture model allows us to make an important reflection concerning relations between quantum and stochastic mechanics. The two theories are sometimes claimed to lead to the same results [Ne] and there are cases when such a claim can be verified. The present model shows that in general there is a principal difference between the two. One can model such a decay in stochastic mechanics too considering random electron trajectories and summing the decay probabilities for their parts situated within the nucleus. The formula is given in [ET92] and we are not going to reproduce it here; what is important that the total probability is expressed as the sum of probabilities of all the contributing processes. In the quantum-mechanical model discussed here, on the other hand, one adds the *amplitudes* – it is obvious from the form factor expression in case of a volume-supported decay – and the total probability is the squared modulus of the sum.

5.3. A model of heavy quarkonia decay

Let us finally mention one more modification of the model, this time aiming at description of decays of charmonium or bottomium, which are bound states of heavy quark-antiquark pairs, into a meson-antimeson pair. Such processes are known to be essentially non-relativistic; as an example one can take the decay $\psi''(3770) \to D\bar{D}$ where the D meson mass is $\approx 1865\,\mathrm{MeV/c}^2$, thus rest energy of the meson pair is two orders of magnitude larger than the kinetic one released in the decay.

If the interaction responsible for the decay is switched off the quark and meson pairs are described by the operators

$$\hat{H}_{0,j} := -\frac{1}{2m_j}\Delta_{j1} - \frac{1}{2m_j}\Delta_{j2} + V_j(|\vec{x}_{j1}-\vec{x}_{j2}|) + 2m_jc^2\,,$$

where m_1 and m_2 are the quark and meson masses, respectively. As before we separate the center-of-mass motion and use the rotational invariance. Adjusting the energy threshold to $2m_2c^2$ we can reduce the problem to investigation of self-adjoint extensions of the operator $H_0^{(\ell)} := H_{0,1}^{(\ell)} \oplus H_{0,2}^{(\ell)}$ on $L^2(R_1,\infty) \oplus L^2(R_2,\infty)$ defined by

$$H_{0,j}^{(\ell)} := -\frac{1}{m_j}\frac{\mathrm{d}^2}{\mathrm{d}r_j^2} + V_j(r_j) + \frac{\ell(\ell+1)}{m_jr_j^2} + 2(m_j-m_2)c^2$$

with $D(H_{0,j}^{(\ell)}) := C_0^\infty(R_j,\infty)$. Let us list the assumptions. We suppose that the quarks can annihilate only they 'hit each other', $R_1 = 0$, while for mesons we allow existence of a hard core, $R_2 = R \geq 0$. One the other hand, the mesons are supposed to be non-interacting, $V_2 = 0$; this may not be realistic if they are charged but it simplifies the treatment. In contrast to that, the interquark potential is *confining*, $\lim_{r\to\infty} V_1(r) = \infty$; we also assume that $V_1 \in L^1_{\mathrm{loc}}$ and a finite $\lim_{r\to 0+} V_1(r)$ exists.

To couple the two channels the deficiency indices of $H_0^{(\ell)}$ have to be $(2,2)$; since we have put $R_1 = 0$ it happens only if $\ell = 0$ and we drop thus the index ℓ in the following. We will not strive again to describe all the extensions and choose a particular one-parameter family: the domain of the extension H_a will consist of functions $f \in W^{2,2}(\mathbb{R}^+) \oplus W^{2,2}(R,\infty)$ satisfying the conditions

$$f_1(0) = a\,f_2'(R)\,, \quad f_2(R) = \frac{m_2}{m_1}\,\bar{a}\,f_1'(0)\,, \tag{5.5}$$

with $a \in \mathbb{C}$. In the decoupled case, $a = 0$, we get Dirichlet boundary condition in both channels as expected; for $a \in \mathbb{R}$ the Hamiltonian is time-reversal invariant.

As the first thing we have to find the resolvent of H_a, in particular its projection to the quark channel. In analogy with the previous section we can write its integral kernel $G_0(r,s;z)$ in terms of two solutions of the equation

$$\Big(-\frac{1}{m_j}\frac{\mathrm{d}^2}{\mathrm{d}r^2} + V_1(r) + 2(m_1-m_2)c^2\Big)f(r) = zf(r)$$

for $z \notin \mathbb{R}$ such that $u(0) = 0$ and v is L^2 at infinity. Krein's formula helps again; by a straightforward computation [AEŠS94] we get

$$G_a(r,s;z) = G_0(r,s;z) + \frac{-ikm_2|a|^2v(r;z)v(s;z)}{m_1v(0;z)D(v,a;z)}\,,$$

where the denominator is given by

$$D(v, a; z) := v(0; z) - ik|a|^2 \frac{m_2}{m_1} v'(0; z)\,.$$

The singularities are again determined by zeros of the last expression. One can work out examples such a natural confining potential, $V_1(r) = \alpha r + V_0 + 2(m_2 - m_1)c^2$, and its modifications, in which the resonance width can be expressed through the value of the quark wave function at the origin. This appears to be the case generally.

Theorem 5.4. [AEŠS94] *Under the stated assumptions, the quarkonium decay width is given for the nth s-wave state by*

$$\Gamma_n(a) = 8\pi k_n \frac{m_2}{m_1^2} |a|^2 |\psi_n(0)|^2 + \mathcal{O}(|a|^6)\,, \quad k_n := \sqrt{m_1 E_n}\,, \tag{5.6}$$

provided the bound-state energy E_n, adjusted by the difference of the rest energies, is positive; $\psi_n(0)$ is the value of the corresponding wave function at the origin.

Note that while we have assumed the quark potential to be below bounded at the origin, the assumption can be relaxed. The theorem holds also for potentials with sufficiently weak singularity, in particular, for the physically interesting case of a linear confinement combined with a Coulomb potential.

6. More about the decay laws

Let us return to the time evolution of unstable systems, in particular, to properties of the decay laws. In addition to the elementary properties mentioned together with the definition (2.1) we know so far only that in the weak-coupling situation they do not differ much from an exponential function coming from the leading term of the pole approximation. This says nothing about local properties of the decay laws which is the topic we are going to investigate in this section.

Historically the first consequence of non-exponentiality associated with the below bounded energy spectrum concerned the long-time behavior of the decay laws; already in [Kh57] it was observed that a sharp energy cut-off leads to the $\mathcal{O}(t^{-3/2})$ behavior as $t \to \infty$, and other examples of that type followed. Moreover, it is even possible that a part of the initial state survives the decay; we have seen a simple example at the end of Sec. 5.1 and another one will be given in Sec. 9 below. Here we concentrate on two other local properties of decay laws.

6.1. Initial decay rate and its implications

The first one concerns the behavior of the system immediately after its preparation. Exponential decay has a constant decay rate which, in particular, means it is nonzero at $t = 0$. This may not be true for other decay laws. We note, for example, that P_ψ is by definition an even function of t, hence if the (two-sided) derivative $\dot{P}_\psi(0)$ exists it has to be zero. This happens for vectors from the form domain of the Hamiltonian: we have $|(\psi, \mathrm{e}^{-iHt}\psi)|^2 \le P_\psi(t) \le 1$ which leads easily to the following conclusion [HE73].

Proposition 6.1. *If $\psi \in Q(H)$ the decay law satisfies $\dot{P}_\psi(0+) = 0$.*

The importance of this result stems from the peculiar behavior of unstable systems subject to frequently repeated measurements knows as *quantum Zeno effect*, namely that in the limit of permanent measurement the system cannot decay. This fact was known essentially already to von Neumann and Turing, in the context of unstable particle decay it was first described by Beskow and Nilsson [BN67] followed by a serious mathematical work [Fr72, Ch] which elucidated the mechanism. It became truly popular, however, only after the flashy name referring to Zeno's aporia about a flying arrow was proposed in [MS77]. Since then the effect was a subject of numerous investigations, in part because it became interesting also from experimental and application points of view. However, since Zeno-type problems are not the subject of this survey we limit ourselves to quoting the review papers [Sch04, FP08] as a guide to further reading, and will discuss the topic only inasmuch it concerns the initial decay rate.

Suppose that we perform on an unstable system a series of measurements at times t/n, $2t/n$, $\dots$, t, in which we ascertain that it is still undecayed. If the outcome of each of them is positive, the state reduction returns the state vector into the subspace $\mathcal{H}_\mathrm{u}$ and the resulting non-decay probability is

$$M_n(t) = P_\psi(t/n) P_{\psi_1}(t/n) \cdots P_{\psi_{n-1}}(t/n)\,,$$

where ψ_{j+1} is the normalized projection of $\mathrm{e}^{-iHt/n}\psi_j$ on $\mathcal{H}_\mathrm{u}$ and $\psi_0 := \psi$, in particular, $M_n(t) = (P_\psi(t/n))^n$ if $\dim \mathcal{H}_\mathrm{u} = 1$ and all the vectors ψ_j coincide with ψ up to a phase factor. Since $\lim_{n\to\infty}(f(t/n)^n = \exp\{-\dot{f}(0+)t\}$ holds whenever $f(0) = 1$ and the one-sided derivative $\dot{f}(0+)$ exists, we see that $\dot{P}_\psi(0+) = 0$ implies the Zeno effect, $M(t) := \lim_{n\to\infty} M_n(t) = 1$ for all $t > 0$, and the same is true if $\dim \mathcal{H}_\mathrm{u} > 1$ provided the derivative $\dot{P}_\psi(0+)$ has such a property for *any* $\psi \in \mathcal{H}_\mathrm{u}$.

At the same time the above simple argument suggests that an opposite situation, an *anti-Zeno effect*, is possible when $\dot{P}_\psi(0+)$ is negative infinite; then $M(t) = 0$ for any $t > 0$ which means that the decay is accelerated and the unstable system disappears once the measurement started. The possibility of such a behavior was mentioned early [CSM77], however, the attention to it is of a recent date only – we refer again to the review work quoted above. Before proceeding further we have to say that the two effects are understood differently in different communities. For experimental physicists the important question is the change of the observed lifetime when the measurement are performed with a certain frequency, on the other hand a theoretical or mathematical physicist typically asks what happens if the period between two successive measurements tends to zero.

Let us return to the initial decay rate. It is clear we have to estimate $1 - P_\psi(t)$ for small values of t, which we can write as $2\,\mathrm{Re}\,(\psi, E_\mathrm{u}(I - \mathrm{e}^{-iHt})\psi) - \|E_\mathrm{u}(I -$

$\mathrm{e}^{-iHt})\psi\|^2$, or alternatively cast it using the spectral theorem into the form

$$4\int_{-\infty}^{\infty}\sin^2\frac{\lambda t}{2}\,\mathrm{d}\|E_\lambda^H\psi\|^2 - 4\left\|\int_{-\infty}^{\infty}\mathrm{e}^{-i\lambda t/2}\,\sin\frac{\lambda t}{2}\,\mathrm{d}E_{\mathrm{u}}E_\lambda^H\psi\right\|^2,$$

where the non-decreasing projection-valued function $\lambda\mapsto E_\lambda^H := E_H((-\infty,\lambda])$ generates spectral measure E_H of the Hamiltonian H. By the Schwarz inequality the above expression is non-negative; we want to find tighter upper and lower bounds.

To this aim we choose an orthonormal basis $\{\chi_j\}$ in the unstable system subspace $\mathcal{H}_{\mathrm{u}}$ and expand the initial state vector as $\psi=\sum_j c_j\chi_j$ with $\sum_j|c_j|^2=1$. The second term in the above expression can then be written as

$$-4\sum_m\left|\sum_j c_j\int_{-\infty}^{\infty}\mathrm{e}^{-i\lambda t/2}\,\sin\frac{\lambda t}{2}\,\mathrm{d}(\chi_m,E_\lambda^H\chi_j)\right|^2,$$

where $\mathrm{d}\omega_{jk}(\lambda) := \mathrm{d}(\chi_j,E_\lambda^H\chi_k)$ are real-valued measures symmetric with respect to interchange of the indices. Since the measure appearing in the first term can be written as $\mathrm{d}\|E_\lambda^H\psi\|^2=\sum_{jk}\bar c_j c_k\mathrm{d}\omega_{jk}(\lambda)$, the decay probability becomes

$$\begin{aligned}1-P_\psi(t) = 4\sum_{jk}\bar c_j c_k\bigg\{&\int_{-\infty}^{\infty}\sin^2\frac{\lambda t}{2}\,d\omega_{jk}(\lambda)\\ &-\sum_m\int_{-\infty}^{\infty}e^{-i\lambda t/2}\,\sin\frac{\lambda t}{2}\,d\omega_{jm}(\lambda)\int_{-\infty}^{\infty}e^{i\mu t/2}\,\sin\frac{\mu t}{2}\,d\omega_{km}(\mu)\bigg\};\end{aligned}$$

if $\dim\mathcal{H}_{\mathrm{u}}=\infty$ the involved series can easily be seen to converge using Parseval's relation. Using next the normalization $\int_{-\infty}^{\infty}\mathrm{d}\omega_{jk}(\lambda)=\delta_{jk}$ we arrive after a simple calculation [Ex05] at the formula

$$1-P_\psi(t) = 2\sum_{jkm}\bar c_j c_k\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\sin^2\frac{(\lambda-\mu)t}{2}\,\mathrm{d}\omega_{jm}(\lambda)\mathrm{d}\omega_{km}(\mu)\,. \tag{6.1}$$

Consider first an upper bound. We fix $\alpha\in(0,2]$ and use the inequalities $|x|^\alpha\ge|\sin x|^\alpha\ge\sin^2 x$ together with $|\lambda-\mu|^\alpha\le 2^\alpha(|\lambda|^\alpha+|\mu|^\alpha)$ to infer that

$$\begin{aligned}\frac{1-P_\psi(t)}{t^\alpha} &\le 2^{1-\alpha}\sum_{jkm}\bar c_j c_k\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}|\lambda-\mu|^\alpha\,\mathrm{d}\omega_{jm}(\lambda)\mathrm{d}\omega_{km}(\mu)\\ &\le 2\sum_{jkm}\bar c_j c_k\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}(|\lambda|^\alpha+|\mu|^\alpha)\,\mathrm{d}\omega_{jm}(\lambda)\mathrm{d}\omega_{km}(\mu)\le 4\langle|H|^\alpha\rangle_\psi\,,\end{aligned}$$

which means that $1-P_\psi(t)=\mathcal{O}(t^\alpha)$ if $\psi\in\mathrm{Dom}\,(|H|^{\alpha/2})$. If this is true for some $\alpha>1$ we get $\dot P_\psi(0+)=0$ which a slightly weaker result than Proposition 6.1. Note also that if $\dim\mathcal{H}_{\mathrm{u}}=1$ and the spectrum of H is absolutely continuous there is an alternative way to justify the claim using the Lipschitz regularity, since $P(t)=|\hat\omega(t)|^2$ in this case and $\hat\omega$ is bounded and uniformly α-Lipschitz *iff* $\int_{\mathbb{R}}\omega(\lambda)(1+|\lambda|^\alpha)\,\mathrm{d}\lambda<\infty$.

A lower bound is more subtle. We use the inequality $\left|\sin\frac{(\lambda-\mu)t}{2}\right| \ge C|\lambda-\mu|t$ which holds with a suitable $C>0$ for $\lambda,\mu\in[-1/t,1/t]$ to estimate (6.1) as follows

$$\begin{aligned}1-P_\psi(t) &\ge 2C^2t^2\int_{-1/t}^{1/t}\int_{-1/t}^{1/t}(\lambda-\mu)^2\,(\psi,\mathrm{d}E_\lambda^H E_\mathrm{u}\mathrm{d}E_\mu^H\psi)\\ &= 4C^2t^2\left\{\int_{-1/t}^{1/t}\int_{-1/t}^{1/t}(\lambda^2-\lambda\mu)\,(\psi,\mathrm{d}E_\lambda^H E_\mathrm{u}\mathrm{d}E_\mu^H\psi)\right\}\\ &= 4C^2t^2\left\{(\psi,H_{1/t}^2E_\mathrm{u}I_{1/t}\psi)-\|PH_{1/t}\psi\|^2\right\},\end{aligned}$$

where H_N denotes the cut-off Hamiltonian, $HE_H(\Delta_N)$ with $\Delta_N:=(-N,N)$. Dividing the expression at the right-hand side by t and choosing $t=N^{-1}$, we arrive at the following conclusion.

Proposition 6.2. *The initial decay rate of $\psi\in\mathcal{H}_\mathrm{u}$ satisfies $\dot{P}_\psi(0+)=-\infty$ provided $\left(\langle H_N^2E_\mathrm{u}E_H(\Delta_N)\rangle_\psi-\|PH_N\psi\|^2\right)^{-1}=o(N)$ holds as $N\to\infty$.*

To illustrate how does the initial decay rate depend on spectral properties of the decaying state, consider an *example* in which $\dim\mathcal{H}_\mathrm{u}=1$, the Hamiltonian is bounded from below and ψ from its absolutely continuous spectral subspace is such that $\mathrm{d}(\psi,E_\lambda^H\psi)=\omega(\lambda)\,\mathrm{d}\lambda$ where $\omega(\lambda)\approx c\lambda^{-\beta}$ as $\lambda\to+\infty$ for some $c>0$ and $\beta>1$. If $\beta>2$, Proposition 6.1 implies $\dot{P}_\psi(0+)=0$. On the other hand, one can easily find the asymptotic behavior of the quantity appearing in Proposition 6.2: $\int_{-N}^{N}\omega(\lambda)\,\mathrm{d}\lambda$ tends to one, while the other two integrals diverge giving

$$\int_{-N}^{N}\lambda^2\,\mathrm{d}\omega(\lambda)\int_{-N}^{N}\mathrm{d}\omega(\lambda)-\left(\int_{-N}^{N}\lambda\,\mathrm{d}\omega(\lambda)\right)^2\approx\frac{c}{3-\beta}N^{3-\beta}-\left(\frac{c}{2-\beta}\right)^2N^{4-2\beta}$$

as $N\to+\infty$, and consequently, $\dot{P}(0+)=-\infty$ holds for $\beta\in(1,2)$. This shows that the exponential decay – which requires, of course, $\sigma(H)=\mathbb{R}$ by Theorem 2.1 – walks a thin line between the two extreme initial-decay-rate possibilities. Let us remark finally that while 'Zeno' limit is trivial for the exponential decay, it may not exist in other cases with $\beta=2$; in [Ex, Rem. 2.4.9] the reader can find an example of such a distribution with a sharp cut-off leading to rapid oscillations of the function $t\mapsto(\psi,\mathrm{e}^{-iHt}\psi)$ which obscure existence of the limit.

6.2. Irregular decay: example of the Winter model

Now we turn to another decay law property. In the literature it is usually tacitly assumed that $P_\psi(\cdot)$ is a 'nice', i.e., sufficiently regular function, typically by dealing with its derivatives. Our aim is to show that this property cannot be taken for granted which we are going to illustrate on another well-known solvable model of decay.

An inspiration comes from the striking behavior of some wave functions in a one-dimensional hard-wall potential well observed in [Be96, Th]. The simplest example concerns the situation when the initial function is constant (and thus not belonging to the domain of the Dirichlet Laplacian): it evolves into a steplike $\psi(x,t)$ for times which are rational multiples of the period, $t = qT$ with $q = N/M$, and the number of steps increases with growing M, while for an irrational q the function $\psi(x,t)$ is fractal with respect to the variable x. One may expect that such a behavior will not disappear completely if the hard wall is replaced by a singular potential barrier. It was illustrated in a 'double well' system [VDS02]; here we instead let the initial state decay into continuum through the tunneling.

Decay due to a barrier tunneling is among the core problem of quantum mechanics which can be traced back to Gamow's paper [Ga28]. The model in which the barrier is a spherical δ-shell is usually referred to as *Winter model* after the paper [Wi61] where it was introduced. A thorough analysis of this model can be found in [AGS87]; it has also various generalizations, we refer to [AGHH] for a bibliography. The Hamiltonian acting in $L^2(\mathbb{R}^3)$ is of the form

$$H_\alpha = -\Delta + \alpha\delta(|\vec{r}| - R)\,, \quad \alpha > 0\,,$$

with a fixed $R > 0$; as usual we employ rational units, $\hbar = 2m = 1$. For simplicity we restrict our attention to the s-wave part of the problem, using the reduced wave functions $\psi(\vec{r},t) = \frac{1}{\sqrt{4\pi}} r^{-1}\phi(r,\, t)$ and the corresponding Hamiltonian part,

$$h_\alpha = -\frac{\mathrm{d}^2}{\mathrm{d}r^2} + \alpha\delta(r - R)\,;$$

we are interested in the time evolution, $\psi(\vec{r},t) = \mathrm{e}^{-iH_\alpha t}\psi(\vec{r},0)$ for a fixed initial condition $\psi(\vec{r},0)$ with the support inside the ball of radius R, and the corresponding decay law $P_\psi(t) = \int_0^R |\phi(r,\, t)|^2\, \mathrm{d}r$ referring to $\mathcal{H}_\mathrm{u} = L^2(B_R(0))$.

It is straightforward to check [AGS87] that H_α has no bound states, on the other hand, it has infinitely many resonances with the widths increasing logarithmically with respect to the resonance index [EF06]; a natural idea is to employ them as a tool to expand the quantities of interest [GMM95]. In order to express reduced evolution in the way described in Section 2 we need to know Green's function of the Hamiltonian h_α which can be obtained from Krein's formula,

$$(h_\alpha - k^2)^{-1}(r,r') = (h_0 - k^2)^{-1}(r,r') + \lambda(k)\Phi_k(r)\Phi_k(r')\,,$$

where $\Phi_k(r) := G_0(r,R)$ is the free Green function with one argument fixed, in particular, $\Phi_k(r) = \frac{1}{k}\sin(kr)\,\mathrm{e}^{ikR}$ holds for $r < R$, and $\lambda(k)$ is determined by δ-interaction matching conditions at $r = R$; by a direct calculation one finds

$$\lambda(k) = -\frac{\alpha}{1 + \frac{i\alpha}{2k}(1 - \mathrm{e}^{2ikR})}\,.$$

Using it we can write the integral kernel of $\mathrm{e}^{-ih_\alpha t}$ as Fourier transformation, $u(t,r,r') = \int_0^\infty p(k,r,r')\mathrm{e}^{-ik^2 t}\, 2k\,\mathrm{d}k$, where the explicit form of the resolvent gives

$$p(k,\, r,\, r') = \frac{2k\sin(kr)\sin(kr')}{\pi(2k^2 + 2\alpha^2\sin^2 kR + 2k\alpha\sin 2kR)}\,.$$

The resonances understood as poles of the resolvent continued to the lower half-plane appear in pairs, those in the fourth quadrant, denoted as k_n in the increasing order of their real parts, and $-\bar{k}_n$; we denote $S = \{k_n,\, -k_n,\, \bar{k}_n,\, -\bar{k}_n \,:\, n \in \mathbb{N}\}$. In the vicinity of k_n the function $p(\cdot, r, r')$ can be written as

$$p(k,r,r') = \frac{i}{2\pi}\frac{v_n(r)v_n(r')}{k^2-k_n^2} + \chi(k,r,r')\,,$$

where $v_n(r)$ solves the differential equation $h_\alpha v_n(r) = k_n^2 v_n(r)$ and χ is locally analytic. It is not difficult to see that the function $p(\cdot, r, r')$ decreases in every direction of the k-plane, hence it can be expressed as the sum over the pole singularities,

$$p(k,r,r') = \sum_{\tilde{k}\in S} \frac{1}{k-\tilde{k}}\, \mathrm{Res}_{\tilde{k}}\, p(k,r,r')$$

and the residue theorem implies $\sum_{\tilde{k}\in S} \mathrm{Res}_{\tilde{k}}\, p(k,r,r') = 0$. Using these relations and denoting $k_{-n} := -\bar{k}_n$ with v_{-n} being the associated solution of the equation $H_\alpha v_{-n}(r) = k_{-n}^2 v_{-n}(r)$, we arrive after a short computation [EF07] at

$$u(t,r,r') = \sum_{n\in\mathbb{Z}} M(k_n,t)v_n(r)v_n(r')$$

with $M(k_n,t) = \frac{1}{2}\,\mathrm{e}^{u_n^2}\,\mathrm{erfc}(u_n)$ and $u_n := -\mathrm{e}^{-i\pi/4}k_n\sqrt{t}$, leading to the decay law

$$P_\psi(t) = \sum_{n,l} C_n \bar{C}_l I_{nl} M(k_n,t)\overline{M(k_l,t)}$$

with $C_n := \int_0^R \phi(r,0)v_n(r)\,\mathrm{d}r$ and $I_{nl} := \int_0^R v_n(r)\bar{v}_l(r)\,\mathrm{d}r$; in our particular case we have $v_n(r) = \sqrt{2}Q_n\sin(k_n r)$ with the coefficient Q_n equal to

$$\left(\frac{-2ik_n^2}{2k_n + \alpha^2 R\sin 2k_nR + \alpha\sin 2k_nR + 2k_n\alpha R\cos 2k_nR}\right)^{1/2}.$$

These explicit formulae allow us to find $P_\psi(t)$ numerically. Let us quote an example worked out in [EF07] in which $R = 1$ and $\alpha = 500$; the initial wave function is chosen to be constant, i.e., the ground state of the *Neumann* Laplacian in $L^2(B_R(0))$ which corresponds to $\phi(r,0) = R^{-3/2}\sqrt{3}r\,\chi_{[0,R]}(r)$.

The respective decay law is plotted in Figure 1; we see that it is irregular having ‘steps’, the most pronounced at the period $T = 2R^2/\pi$ and its simple rational multiples. This is made even more visible from the plot of its logarithmic derivative (for numerical reasons it is locally smeared, otherwise the picture would be a fuzzy band). It is reasonable to conjecture that the function is in fact *fractal.*

Let us add a few heuristic considerations in favor of this conjecture concerning the behavior of the derivative in the limit $\alpha \to \infty$. We can write the wave function as $\phi(r,t) \approx \sum_n c_n \exp(-ik_n^2 t)v_n(r)$ where resonance position expands for a fixed n around $k_{n,0} := n\pi/R$ as $k_n \approx k_{n,0} - k_{n,0}(\alpha R)^{-1} + k_{n,0}(\alpha R)^{-2} - ik_{n,0}^2(\alpha^2 R)^{-1}$. In the leading order we have $v_n(r) \approx \sqrt{\frac{2}{R}}\sin(k_n r)$ and the substantial contribution to the expansion of $\phi(r,t)$ comes from terms with $n \lesssim [\alpha^{1-\varepsilon}\frac{R}{\pi}]$ for some $0 < \varepsilon < 1/3$.

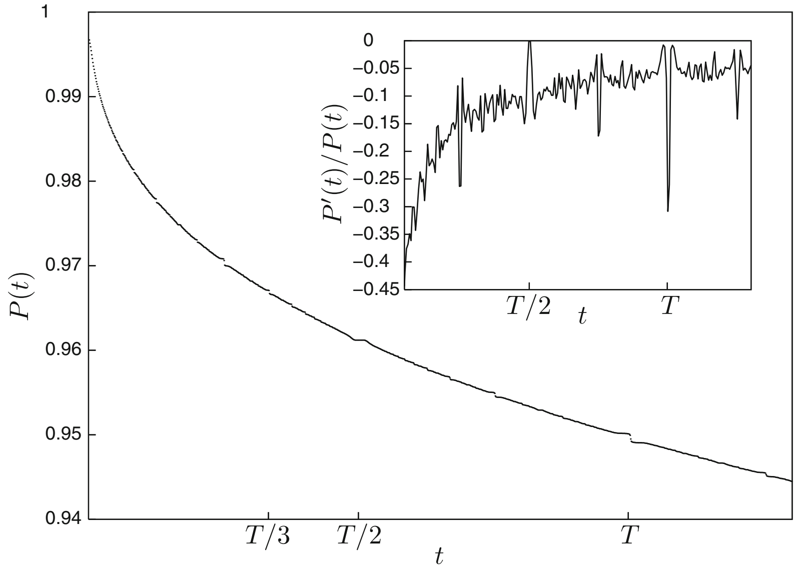

FIGURE 1. Decay law for the initial state $\phi(r,0) = R^{-3/2}\sqrt{3}r$; the inset shows its logarithmic derivative averaged over intervals of the length approximately $T/200$.

The derivative of the decay law $P_{\psi,\alpha}(\cdot)$ can be identified with the probability current through the sphere, $\dot{P}_{\psi,\alpha}(t) = -2\mathrm{Im}\,(\phi'(R,t)\bar{\phi}(R,t))$. To use it we have to know the expressions on the right-hand side; using the above expansion we find

$$\phi(R,t) \approx \sqrt{\frac{2}{R}}\sum_{n=1}^{\infty}(-1)^n c_n \mathrm{e}^{-ik_{n,0}^2 t\left(1-\frac{2}{\alpha R}\right)}\mathrm{e}^{-\frac{2k_{n,0}^3}{\alpha^2 R}t}\left(-\frac{k_{n,0}}{\alpha} - i\frac{k_{n,0}^2}{\alpha^2}\right)$$

and a similar expansion for $\phi'(R,t)$ with the last bracket replaced by $k_{n,0}$. We observe that $\sum_{n=1}^{\infty}\exp\left(-2\frac{k_{n,0}^3}{\alpha^2 R}t\right)k_{n,0}^j \approx \frac{R}{\pi}\left(\frac{R}{2t}\right)^{(j+1)/3}\alpha^{2(j+1)/3}I_j$ holds for $j > -1$ where on the right-hand side we have denoted $I_j := \int_0^\infty \mathrm{e}^{-x^3}x^j\,\mathrm{d}x = \frac{1}{3}\Gamma\left(\frac{j+1}{3}\right)$.

Using this result we can argue that the decay law regularity depends on the asymptotic behavior of the coefficients c_n. Suppose for simplicity that it is power-like, $c_n = \mathcal{O}(k_{n,0}^{-p})$ as $n \to \infty$. If the decay is fast enough, $p > 1$, we find that $|\dot{P}_{\psi,\alpha}(t)| \leq \mathrm{const}\,\alpha^{4/3-4/3p} \to 0$ holds as $\alpha \to \infty$ uniformly in the time variable. The situation is different if the decay is slow, $p \leq 1$. Consider the example mentioned above leading to the decay law featured in Figure 1 where $c_n = (-1)^{n+1}\frac{\sqrt{6}}{Rk_n}$. Since the real parts of the resonance poles change with α, it is natural to look at the limit of $\dot{P}_{\psi,\alpha}(t_\alpha)$ as $\alpha \to \infty$ at the moving time value $t_\alpha := t(1 + 2/\alpha R)$.

For irrational multiples of T we use the fact [BG88] that the modulus of $\sum_{n=1}^{L} \mathrm{e}^{i\pi n^2 t}$ is for an irrational t bound by $C\, L^{1-\varepsilon}$ where C, ε depend on t only. In combination with the estimate, $\sum_{n=1}^{\infty} a_n b_n \le \sum_{n=1}^{\infty} |\sum_{j=1}^{n} a_j|\, |b_n - b_{n+1}|$ we find

$$\sum_{n=1}^{\infty} \mathrm{e}^{-ik_{n,0}^2 t}\, \mathrm{e}^{-\frac{2k_{n,0}^2}{\alpha^2 R} t} k_{n,0}^{j} \lesssim \mathrm{const}\, \alpha^{2/3(j+1-\varepsilon)}\,,$$

and consequently, $\dot{P}_{\psi,\alpha}(t_\alpha) \to 0$ as $\alpha \to \infty$. Assume next that $t = \frac{p}{q} T$ with $p, q \in \mathbb{N}$. If pq is odd then $S_L(t) := \sum_{n=1}^{L} \mathrm{e}^{i\pi n^2 t}$ repeatedly retraces according to [BG88] the same pattern, hence $\dot{P}_{\psi,\alpha}(t_\alpha) \to 0$ – an illustration can be seen in Fig. 1 at the half-period. On the other hand, for pq even $|S_L(t)|$ grows linearly with L, and consequently, $\lim_{\alpha\to\infty} \dot{P}_{\psi,\alpha}(t_\alpha) > 0$. For instance, a direct computation [EF07] yields the value at the period, $\lim_{\alpha\to\infty} \dot{P}_{\psi,\alpha}(T_\alpha) = -\frac{4}{3\sqrt{3}} \approx -0.77$.

As the last remark in this section, we note that there is a relation between a lack of local regularity of the decay law and the 'anti-Zeno' property of Proposition 6.2; both occur if the energy distribution of the decaying state has a slow enough decay at high energies. The connection is no doubt worth of further exploration.

7. Quantum graphs

Many quantum systems, both spontaneously emerging in nature and resulting from an experimentalist's design, no doubt intelligent one, have complicated geometrical and topological structure which can be conveniently modeled as a graph to which the particle motion is confined. Such a concept was first developed for the purpose of quantum chemistry [RS53], however, it became a subject of intense investigation only at the end of the 1980's when tiny graph-like structures of semiconductor and other materials gained a prominent position in experimental physics. The literature on quantum graphs is vast at present; we limit ourselves with referring to the proceedings volume [EKKST] as a guide for further reading.

Quantum graphs are usually rich in resonances; the reason, as we see below, is that their spectra often exhibit embedded eigenvalues which, as we know, are typically sources of resonance effects. Before we turn to the review let us briefly mention that while describing real-world quantum system through graphs is certainly an idealization, they can be approximated by more realistic 'fat-graph' structures in a well-defined mathematical sense; from our point of view here it is important than such approximations also include convergence of resonances [EP07].

7.1. Basic notions

As a preliminary, let us recall some basic notions about quantum graph models we shall need in the following. For the purpose of this review, a graph Γ consists of a set of vertices $\mathcal{V} = \{\mathcal{X}_j : j \in I\}$, a set of finite edges[2] $\mathcal{L} = \{\mathcal{L}_{jn} : (\mathcal{X}_j, \mathcal{X}_n) \in I_{\mathcal{L}} \subset I \times I\}$, and a set of infinite edges, sometimes also called *leads*, $\mathcal{L}_\infty = \{\mathcal{L}_{j\infty} : \mathcal{X}_j \in I_{\mathcal{C}}\}$ attached to them. The index sets I, $I_{\mathcal{L}}\, I_{\mathcal{C}}$ labeling the vertices and the edges of both types are supposed to be at most countable.

We consider *metric* graphs which means that each edge of Γ is isomorphic to a line segment; the notions of finiteness or (semi)infiniteness refer to the length of those segments. Without loss of generality we may identify the latter with the intervals $(0, l_j)$, where l_j is the jth edge length, and $(0, \infty)$, respectively. As indicated, we regard Γ as the configuration space of a quantum system and with the above convention in mind we associate with it the Hilbert space

$$\mathcal{H} = \bigoplus_{\mathcal{L}_j \in \mathcal{L}} L^2([0, l_j]) \oplus \bigoplus_{\mathcal{L}_{j\infty} \in \mathcal{L}_\infty} L^2([0, \infty))\,,$$

the elements of which are columns $\Psi = (\{f_j : \mathcal{L}_j \in \mathcal{L}\},\, \{g_j : \mathcal{L}_{j\infty} \in \mathcal{L}_\infty\})^{\mathrm{T}}$.

For most part of this section we will suppose that the motion on the graph edges is free, i.e., governed by the Hamiltonian which acts there as $-\frac{\mathrm{d}^2}{\mathrm{d}x^2}$ with respect to the arc-length variable parametrizing of the particular edge. In such a case we have a limit-circle situation at the edge endpoints, hence in order to make it a self-adjoint operator, we have to impose appropriate boundary conditions which couple the wave functions at the graph vertices. One of the possible general forms of such conditions [GG, Ha00, KS00] is

$$(U_j - I)\Psi_j + i(U_j + I)\Psi'_j = 0\,, \tag{7.1}$$

where U_j are unitary matrices, and Ψ_j and Ψ'_j are vectors of the functional values and of the (outward) derivatives at the vertex $\mathcal{X}_j$; in other words, the domain of the Hamiltonian consists of all functions on Γ which are locally $W^{2,2}$ and satisfy conditions (7.1). It is easy to see that the conditions (7.1) ensure vanishing of the appropriate boundary form, namely

$$\sum_{k=1}^{\deg \mathcal{X}_j} (\bar{\psi}_{jk}\psi'_{jk} - \bar{\psi}'_{jk}\psi_{jk})(0) = 0$$

with $\Psi_j = \{\psi_{jk}\}$ and $\Psi'_j = \{\psi'_{jk}\}$, or, in physical terms, conservation of the probability current at the junction. Note that coupling we have introduced here is local connecting boundary values in a single vertex $\mathcal{X}_j$ only.

Since handling Hamiltonians of graphs with a complicated topology may be cumbersome, one can simplify treatment of such cases using a trick proposed first in [Ku08]. It consists of replacing Γ with the graph Γ_0 in which all edge ends meet in a single vertex as sketched in Figure 2; the actual topology of the original graph Γ will be then encoded into the matrix which describes the coupling in such a 'grand' vertex. Denoting $N = \sharp\,\mathcal{L}$ and $M = \sharp\,\mathcal{L}_\infty$ we introduce the $(2N + M)$-dimensional

[2] We assume here implicitly that any two vertices are connected by not more than a single edge and that the graph has no loops, which is possible to do without loss of generality since we are always able to insert 'dummy' vertices into 'superfluous' edges.

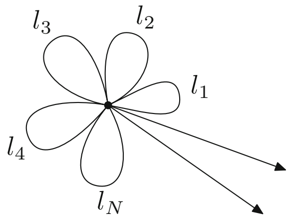

FIGURE 2. The model Γ_0 for a quantum graph Γ with N internal finite edges and M external leads.

vector of functional values by $\Psi = (\Psi_1^T, \dots, \Psi_{\sharp\mathcal{V}}^T)^T$ and similarly the vector of derivatives Ψ' at the vertex; the conditions (7.1) can be concisely rewritten as coupling on Γ_0 characterized by $(2N+M)\times(2N+M)$ unitary block-diagonal matrix U, consisting of the blocks U_j, in the form

$$(U-I)\Psi + i(U+I)\Psi' = 0\,; \tag{7.2}$$

it is obvious that one can treat the replacement as a unitary equivalence which does not alter spectral properties and preserves the system resonances (if there are any).

7.2. Equivalence of resonance notions

In Section 2 we made it clear how important it is to establish connection between different objects labeled as resonances. Let us look now how this question looks like in the quantum graph setting. Let us begin with the resolvent resonances. One can write the resolvent of the graph Hamiltonian [Pa10], however, it is sufficient to inspect the spectral condition encoded in it and its behavior in the complex plane.

We employ an external complex scaling in which the external part are the semi-infinite leads where the functions are scaled as $g_{j\theta}(x) = \mathrm{e}^{\theta/2} g_j(x\mathrm{e}^{\theta})$ with an imaginary θ; as usual this rotates the essential spectrum of the transformed (non-selfadjoint) Hamiltonian into the lower complex half-plane and reveals the second-sheet poles. In particular the 'exterior' boundary values, to be inserted into (7.2), can be for $g_j(x) = c_j\,\mathrm{e}^{ikx}$ written as $g_j(0) = \mathrm{e}^{-\theta/2} g_{j\theta}$ and $g_j'(0) = ik\mathrm{e}^{-\theta/2} g_{j\theta}$ with an appropriate $g_{j\theta}$. On the other hand, the internal part of the graph is left unscaled. Choosing the solution on the jth edge in the form $f_j(x) = a_j \sin kx + b_j \cos kx$ we easily find its boundary values; for $x=0$ it is trivial, for $x = l_j$ we use the standard transfer matrix. This allows us to express both $(f_j(0), f_j(l_j))^{\mathrm{T}}$ and $(f_j'(0), -f_j'(l_j))^{\mathrm{T}}$ through the coefficients a_j, b_j, cf. [EL10] and note the sign of $f_j'(l_j)$ reflecting the fact that the derivatives entering (7.2) are outward ones.

Inserting these boundary values into the coupling condition we arrive at the system

$$(U-I)C_1(k)\begin{pmatrix} a_1 \\ b_1 \\ a_2 \\ \vdots \\ b_N \\ \mathrm{e}^{-\theta/2}g_{1\theta} \\ \vdots \\ \mathrm{e}^{-\theta/2}g_{M\theta} \end{pmatrix} + ik(U+I)C_2(k)\begin{pmatrix} a_1 \\ b_1 \\ a_2 \\ \vdots \\ b_N \\ \mathrm{e}^{-\theta/2}g_{1\theta} \\ \vdots \\ \mathrm{e}^{-\theta/2}g_{M\theta} \end{pmatrix} = 0, \qquad (7.3)$$

where we have set $C_1(k) = \mathrm{diag}\,(C_1^{(1)}(k), C_1^{(2)}(k), \dots, C_1^{(N)}(k), I_{M\times M})$ and $C_2 = \mathrm{diag}\,(C_2^{(1)}(k), C_2^{(2)}(k), \dots, C_2^{(N)}(k), iI_{M\times M})$ with

$$C_1^{(j)}(k) = \begin{pmatrix} 0 & 1 \\ \sin kl_j & \cos kl_j \end{pmatrix}, \quad C_2^{(j)}(k) = \begin{pmatrix} 1 & 0 \\ -\cos kl_j & \sin kl_j \end{pmatrix},$$

and $I_{M\times M}$ being the $M \times M$ unit matrix. The solvability condition of the system (7.3) determines eigenvalues of the scaled non-selfadjoint operator, and *mutatis mutandis*, poles of the analytically continued resolvent of the original Hamiltonian.

Looking at the same system from the scattering point of view we use the same solution as above on the internal edges while on the leads we take appropriate combinations of two planar waves, $g_j = c_j\mathrm{e}^{-ikx} + d_j\mathrm{e}^{ikx}$. We look for the on-shell S-matrix $S = S(k)$ which maps the vector of amplitudes of the incoming waves $c = \{c_n\}$ into the vector of amplitudes of the outgoing waves $d = \{d_n\}$, and ask about its complex singularities, $\det S^{-1} = 0$. This leads to the system

$$(U-I)C_1(k)\begin{pmatrix} a_1 \\ b_1 \\ a_2 \\ \vdots \\ b_N \\ c_1+d_1 \\ \vdots \\ c_M+d_M \end{pmatrix} + ik(U+I)C_2(k)\begin{pmatrix} a_1 \\ b_1 \\ a_2 \\ \vdots \\ b_N \\ d_1-c_1 \\ \vdots \\ d_M-c_M \end{pmatrix} = 0\,;$$

eliminating the variables a_j, b_j one can rewrite it as a system of M equations expressing the map $S^{-1}d = c$. The condition under which the latter is not solvable, which is equivalent to our original question since S is unitary, reads

$$\det\,[(U-I)\,C_1(k) + ik(U+I)\,C_2(k)] = 0\,, \qquad (7.4)$$

however, this is nothing else than the condition of solvability of the system (7.3). This is the core of the argument leading us to the following conclusion [EL10].

Theorem 7.1. *The notions of resolvent and scattering resonances coincide for quantum graph Hamiltonians described above.*

Before proceeding further, let us mention one more way in which the resonance problem on a graph can be reformulated. To this purpose we rearrange the matrix U permuting its rows and columns into the form $U = \begin{pmatrix} U_1 & U_2 \\ U_3 & U4 \end{pmatrix}$, where U_1 is the $2N \times 2N$ square matrix referring to the compact subgraph, U_4 is the $M \times M$ square matrix related to the exterior part, and U_2 and U_3 are rectangular matrices of the size $M \times 2N$ and $2N \times M$, respectively, connecting the two. The system (7.3) can then be rewritten by elimination of the lead variables [EL10] as

$$(\tilde{U}(k) - I)F + i(\tilde{U}(k) + I)F' = 0\,, \tag{7.5}$$

where $F := (f_1, \dots, f_{2N})^{\mathrm{T}}$, and similarly for F', are the internal boundary values, and the effective coupling matrix appearing in this condition is given by

$$\tilde{U}(k) = U_1 - (1-k)U_2[(1-k)U_4 - (k+1)I]^{-1}U_3\,. \tag{7.6}$$

In other words, we have been able to cast the problem into the form of spectral question for the compact core of the graph with the effective coupling replacing the leads by the non-unitary and energy-dependent matrix (7.6).

7.3. Line with a stub

Next we will present several simple examples. In the first one Γ is a line to which a segment is attached at the point $x = 0$. The Hilbert space is thus $\mathcal{H} := L^2(\mathbb{R}) \oplus L^2(0,l)$ and we write its elements as columns $\psi = \binom{f}{u}$. To make the problem more interesting we suppose that the particle on the stub is exposed to a potential; the Hamiltonian acts

$$(H\psi)_1(x) = -f''(x)\,, \quad (H\psi)_2(x) = (-u'' + Vu)(x)\,,$$

outside the junction, where $V \in L^1_{\mathrm{loc}}(0,l)$ having finite limits at both endpoints of the segment so – if the domain consists of functions vanishing in the vicinity of the junction – the corresponding deficiency indices are $(3,3)$. The admissible Hamiltonians will be identified with self-adjoint extensions which, as before, can be conveniently characterized by appropriate boundary conditions. We will not explore all of them and restrict our attention to a subclass of those having the line component of the wave function continuous at the junction, namely

$$\begin{aligned} f(0+) = f(0-) =: f(0)\,, \qquad & u(0) = bf(0) + cu'(0)\,, \\ f'(0+) - f'(0-) = df(0) - bu'(0)\,, \qquad & u(\ell) = 0\,; \end{aligned} \tag{7.7}$$

at the free end of the stub we fix the Dirichlet condition. The coefficient matrix $\mathcal{K} = \begin{pmatrix} b & c \\ d & -b \end{pmatrix}$ is real; we restrict our attention to time-reversal invariant dynamics. The operator specified by the conditions (7.7) will be denoted as $H_{\mathcal{K}}$. The parameter b controls the coupling; if $b = 0$ the graph decomposes into the line with a point interaction at $x = 0$ and the stub supporting the Schrödinger operator $h_c := -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V$ with Robin condition $u(0) = cu'(0)$ at the junction referring again to $x = 0$.

Let us begin with the scattering. To find the on-shell S-matrix we use the standard Ansatz, $f(x) = \mathrm{e}^{ikx} + r\,\mathrm{e}^{-ikx}$ and $t\,\mathrm{e}^{ikx}$ on the line for $x < 0$ and $x > 0$, respectively, while on the stub we take $u(x) = \beta u_l(x)$ where u_l is a solution to

$-u'' + Vu = k^2 u$ corresponding to the boundary conditions $u_l(l) = 0$, unique up to a multiplicative constant. Using the coupling conditions (7.7) we find

$$t(k) = \frac{-2ik(cu'_\ell - u_\ell)(0)}{2ikD(k)}, \quad r(k) = -\frac{b^2 u'_\ell(0) + d(cu'_\ell - u_\ell)(0)}{2ikD(k)};$$

where $2ikD(k) := b^2 u'_\ell(0) + (d - 2ik)(cu'_\ell - u_\ell)(0)$; it is easy to check that these amplitudes satisfy $|t(k)|^2 + |r(k)|^2 = 1$. We note that $H_\mathcal{K}$ can have also an isolated eigenvalue; this happens if $D(i\kappa) = 0$ with $\kappa > 0$. If $b = 0$ such an eigenvalue exists provided $d < 0$ and equals $-\frac{1}{4}d^2$; it remains isolated for $|b|$ small enough.

It is also not difficult to find the resolvent of $H_\mathcal{K}$. The tool is as usual Krein's formula; we choose for comparison $H_{\mathcal{K}_0}$ corresponding to $\mathcal{K}_0 = 0$. In that case the operator decomposes, the kernel of line part being $G_1(x, y; z) = \frac{i}{2k}\, e^{ik|x-y|}$ where $k := \sqrt{z}$ as usual; the stub part is $-\frac{u_0(x_<)u_\ell(x_>)}{W(u_0,u_l)}$, where u_l has been introduced above, u_0 is similarly a solution corresponding to the condition $u_0(0) = cu'_0(0)$, and $W(u_0, u_l)$ is the Wronskian of the two functions. The sought kernel then equals

$$(H_\mathcal{K} - z)^{-1}(x, y) = (H_{\mathcal{K}_0} - z)^{-1}(x, y) + \sum_{j=1,2} \lambda_{jk}(k) F_j(x) F_k(y),$$

where the vectors F_j can be chosen as $F_1(x) := \binom{R_1(x,0)}{0}$ and $F_2(x) := \binom{0}{u_l(x)}$; note that the stub part vanishes at $x = 0$. The coefficients are obtained from the requirement that the resolvent must map any vector of $\mathcal{H}$ into the domain of $H_\mathcal{K}$; a straightforward computation [EŠ94] gives

$$\lambda_{11}(k) = \frac{b^2 u'_\ell(0) + d(cu'_\ell - u_\ell)(0)}{D(k)}, \quad \lambda_{22}(k) = \frac{u_\ell(0)^{-1}}{D(k)} \left(c + i\, \frac{cd + b^2}{2k} \right),$$

together with $\lambda_{12}(k) = \lambda_{21}(k) = bD(k)^{-1}$. We see, in particular, that the coefficient denominator zeros in the complex plane coincide with those of the on-shell S-matrix as we expect based on Theorem 7.1 proved above.

In the decoupled case, $b = 0$, the expression for $D(k)$ factorizes giving rise to eigenvalues of the operator h_c introduced above which are embedded in the continuous spectrum of the line Hamiltonian; the coupling turns them generally into resonances. In the case case of weak coupling, i.e., for small $|b|$ one can solve the condition $D(k) = 0$ perturbatively arriving at the following conclusion [EŠ94].

Proposition 7.2. *Let k_n refer to the nth eigenvalue of h_c and denote by χ_n the corresponding normalized eigenfunction; then for all sufficiently small $|b|$ there is a unique resolvent pole in the vicinity of k_n given by*

$$k_n(b) = k_n - \frac{ib^2 \chi'_n(0)^2}{2k_n(2k_n + id)} + \mathcal{O}(b^4).$$

This gives, in particular, the inverse value of resonance lifetime in the weak-coupling case, $\mathrm{Im}\, z_n(b) = ib^2 \chi'_n(0)^2 (2k_n + id)^{-1} + \mathcal{O}(b^4)$. The simple form of the condition $D(k) = 0$ allows us, however, to go beyond the weak coupling and to trace numerically the pole trajectories as the coupling constant b runs over the reals. Examples are worked out in [EŠ94] but we will not describe them here and limit ourselves with mentioning an important particular situation.

It concerns the case when the motion in the stub is free and the decoupled operator is specified by the Dirichlet boundary condition, i.e., $V = 0$ and $c = d = 0$. The condition $D(k) = 0$ can then be solved analytically. Indeed, the embedded eigenvalues are k_n^2 with $k_n := \frac{n\pi}{\ell}$ and the equation reduces to $\tan k\ell = -\frac{i\beta^2}{2}$ solved by

$$k_n(b) = \begin{cases} \frac{n\pi}{\ell} + \frac{i}{2l} \ln \frac{2-b^2}{2+b^2} & \dots \quad |b| < \sqrt{2} \\ \frac{(2n-1)\pi}{2\ell} + \frac{i}{2l} \ln \frac{b^2-2}{b^2+2} & \dots \quad |b| > \sqrt{2} \end{cases} \tag{7.8}$$

Hence the poles move with the increasing $|b|$ vertically down in the k-plane and for $|b| > \sqrt{2}$ they ascend, again vertically, returning to eigenvalues of Neumann version of h_c as $|b| \to \infty$. An important conclusion from this example is that poles may disappear to infinite distance from the real axis and a quantum graph may have no resonances at all, as it happens here for $|b| = \sqrt{2}$.

7.4. Regeneration in decay: a lasso graph

Let us next describe another simple example, now with a lasso-shaped Γ consisting of a circular loop of radius R to which a half-line lead is attached. This time we shall suppose that the particle is charged and the graph is placed into a homogeneous magnetic field of intensity B perpendicular to the loop plane[3]. The vector potential can then be chosen tangent to the loop with the modulus $A = \frac{1}{2}\, BR = \frac{\Phi}{L}$, where Φ is the flux through the loop and L is its perimeter. With the convention we use, $e = c = 2m = \hbar = 1$, the natural flux unit is $\frac{hc}{e} = 2\pi$, so we can also write $A = \frac{\phi}{R}$ where ϕ is the flux value in these units. The Hilbert space of the lasso-graph model is $\mathcal{H} := L^2(0, L) \oplus L^2(\mathbb{R}^+)$; the wave functions are written as columns, $\psi = \binom{u}{f}$.

To construct the Hamiltonian we begin with the operator describing the free motion on the loop and the lead under the assumption that the graph vertex is 'fully disconnected', in other words $H_\infty = H_{\text{loop}}(B) \oplus H_{\text{half-line}}$, where

$$H_{\text{loop}}(B) = \Big(-i\frac{\mathrm{d}}{\mathrm{d}x} + A \Big)^2, \quad H_{\text{half-line}} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2}$$

with Dirichlet condition, $u(0) = u(L) = f(0) = 0$ at the junction. The spectrum of H_{loop} is discrete of multiplicity two; the eigenfunctions $\chi_n(x) = \frac{\mathrm{e}^{-iAx}}{\sqrt{\pi R}} \sin\left(\frac{nx}{2R}\right)$ with $n = 1, 2, \dots$ correspond to the eigenvalues $\left(\frac{n}{2R}\right)^2$ which are embedded into the continuous spectrum of $H_{\text{half-line}}$ covering the interval $[0, \infty)$; note that the effect of the magnetic field on the *disconnected* loop amounts to a unitary equivalence, $H_{\text{loop}}(B) = U_{-A} H_{\text{loop}}(0) U_A$ where $(U_A u)(x) := \mathrm{e}^{iAx} u(x)$.

Restricting the domain of H_∞ to functions vanishing in the vicinity of the junction we get a symmetric operator with deficiency indices $(3, 3)$. We are going

[3]The assumptions of homogeneity and field direction are here for simplicity only, in fact the only thing which matters in the model is the magnetic flux through the loop.

to consider a subclass of its self-adjoint extensions analogous to (7.7) characterized by three real parameters; the Hamiltonian will act as

$$H_{\alpha,\mu,\omega}(B)\begin{pmatrix}u\\ f\end{pmatrix}=\begin{pmatrix}-u''-2iAu'+A^2u\\ -f''\end{pmatrix}$$

on functions from $W^{2,2}_{\mathrm{loc}}(\Gamma)$ continuous on the loop, $u(0)=u(L)$, which satisfy

$$f(0)=\omega u(0)+\mu f'(0)\,,\quad u'(0)-u'(L)=\alpha u(0)-\omega f'(0)\,, \tag{7.9}$$

for some $\alpha,\mu,\omega\in\mathbb{R}$ the latter being the coupling constant. This includes a particular case of *δ-coupling* corresponding to $\mu=0$ and $\omega=1$ in which case the wave functions are fully continuous,

$$u(0)=u(L)=f(0)\,,\quad u'(0)-u'(L)+f'(0)=\alpha f(0)\,; \tag{7.10}$$

in the fully decoupled case we have $\alpha=\infty$ as the notation suggests. For simplicity we will write $H_{\alpha,0,1}=H_\alpha$. Note that in general the vector potential enters the coupling conditions [KS03] but here the outward tangent components of $\vec{A}$ at the junction have opposite signs so their contributions cancel mutually.

Let us start again with scattering, i.e., the reflection of the particle traveling along the half-line from the magnetic-loop end. To find the generalized eigenvectors, $H_{\alpha,\mu,\omega}(B)\psi=k^2\psi$, we use $u(x)=\beta\,\mathrm{e}^{-iAx}\sin(kx+\gamma)$ and $f(x)=\mathrm{e}^{-ikx}+r\,\mathrm{e}^{ikx}$ as the Ansatz; using the coupling conditions (7.9) we get after a simple algebra

$$r(k)=-\frac{(1+ik\mu)\left[\alpha-\frac{2k}{\sin kL}\left(\cos\Phi-\cos kL\right)\right]+i\omega^2k}{(1-ik\mu)\left[\alpha-\frac{2k}{\sin kL}\left(\cos\Phi-\cos kL\right)\right]-i\omega^2k}$$

for the reflection amplitude. The Hamiltonian $H_{\alpha,\mu,\omega}(B)$ can have also isolated eigenvalues but we shall skip this effect referring to [Ex97]. On the other hand, it is important to mention that there may exist *positive* eigenvalues embedded in the continuous spectrum even if $\omega\neq 0$. In view of (7.9) it is possible if $u(0)=u'(0)-u'(L)=0$, hence such bound states exist only at integer/half-integer values of the magnetic flux (in the natural units) and the corresponding eigenfunctions are the χ_n's mentioned above with even n for ϕ integer and odd n for ϕ half-integer.

Next we find the resolvent of $H_{\alpha,\mu,\omega}(B)$ using again Krein's formula to compare it to that of H_∞ with the kernel

$$\mathrm{diag}\left(\mathrm{e}^{-iA(x-y)}\,\frac{\sin kx_<\sin k(x_>-L)}{k\,\sin kL},\;\frac{\sin kx_<\,\mathrm{e}^{ikx_>}}{k}\right).$$

The sought resolvent kernel can then be written as

$$G_{\alpha,\mu,\omega}(x,y;k)=G_\infty(x,y;k)+\sum_{j,\ell=1}^{2}\lambda_{j\ell}(k)F_j(x)F_\ell(y)\,,$$

where the deficiency subspaces involved are chosen in the form

$$F_1(x):=\begin{pmatrix}w(x)\\ 0\end{pmatrix},\qquad F_2(x):=\begin{pmatrix}0\\ e^{ikx}\end{pmatrix}$$

with $w(x) := e^{iAx}\,\frac{e^{-i\Phi}\sin kx - \sin k(x-L)}{\sin kL}$ and the coefficients $\lambda_{j\ell}(k)$ given by [Ex97]

$$\lambda_{11} = -\frac{1-i\mu k}{D(k)}\,, \quad \lambda_{22} = \frac{\mu\left[2k\,\frac{\cos\Phi - \cos kL}{\sin kL} - \alpha\right] - \omega^2}{D(k)}$$

together with $\lambda_{12} = \lambda_{21} = -\frac{\omega}{D(k)}$, where

$$D(k) \equiv D(\alpha, \mu\,\omega; k) := (1-i\mu k)\left[2k\,\frac{\cos\Phi - \cos kL}{\sin kL} - \alpha\right] - i\omega^2 k\,.$$

In the case of a δ-coupling, in particular, the coefficients acquire a simple form, $\lambda_{jl}(k) = -D(k)^{-1}$, $j,l = 1,2$. As expected, the denominator $D(k)$ determining the singularities is the same as for the on-shell S-matrix. A simple form of the condition $D(k) = 0$ allows us to follow the pole trajectories, both with respect to the coupling parameters and the flux Φ. At the same time, knowing the resolvent of $H_{\alpha,\mu,\omega}(B)$ we can express the decay law for states supported at the initial moment $t = 0$ on the loop only; we will not go into details and refer the reader to [Ex97] where the appropriate formulae and plots are worked out.

Let us just mention one amusing feature of this model which can be regarded as an analogue of the effect known in particle physics as *regeneration* in decay of neutral kaons and illustrates that intuition may misguide you when dealing with quantum systems. Consider the lasso graph with the initial wave function u on the loop such that $x \mapsto \mathrm{e}^{iAx}u(x)$ has no definite symmetry with respect to the connection point $x = 0$. If the flux value ϕ is integer, the A-even component represents a superposition of embedded-eigenvalue bound states mentioned above, thus it survives, while the A-odd one dies out. Suppose that after a sufficiently long time we decouple the lead and attach it at a different point (or we may have a loop with two leads which may be switched on and off independently). For the decay of the surviving state the symmetry with respect to the new junction is important; from this point of view it is again a superposition of an A-even and an A-odd part, possibly even with same weights if the distance between the two junctions is $\frac{1}{4}L$.

7.5. Resonances from rationality violation

The above simple examples illustrated that resonances are a frequent phenomenon in quantum graph models. To underline this point we shall describe in this section another mechanism giving rise to resonances, this time without need to change the coupling parameters. The observation behind this claim is that quantum-graph Hamiltonians may have embedded eigenvalues even if no edges are disconnected which is related to the fact that the unique continuation principle is generally not valid here and one can have compactly supported eigenfunctions. Indeed, eigenfunctions of a graph Laplacian are trigonometric functions, hence it may happen that the graph has a loop and the vertices on it have rationally related distances such that the eigenfunction has zeros there and the rest of the graph 'does not know' about it. Let us present briefly two such examples referring to [EL10] for more details.

7.5.1. A loop with two leads. In this case Γ consists of two internal edges of lengths l_1, l_2 and one half-line attached at each of their endpoints, corresponding to the Hilbert space is $L^2(\mathbb{R}^+)\oplus L^2(\mathbb{R}^+)\oplus L^2([0,l_1])\oplus L^2([0,l_2])$; states of the system are correspondingly described by columns $\psi=(g_1,g_2,f_1,f_2)^{\mathrm{T}}$. The Hamiltonian H is supposed to act as negative Laplacian, $\psi\mapsto -\psi''$, separately on each edge. We consider coupling analogous to (7.7) assuming that the functions of $\operatorname{Dom} H$ are continuous on the loop, $f_1(0)=f_2(0)$ and $f_1(l_1)=f_2(l_2)$, and satisfy

$$f_1(0)=\alpha_1^{-1}(f_1'(0)+f_2'(0))+\gamma_1 g_1'(0)\,,\;\; f_1(l_1)=-\alpha_2^{-1}(f_1'(l_1)+f_2'(l_2))+\gamma_2 g_2'(0)\,,$$
$$g_1(0)=\gamma_1(f_1'(0)+f_2'(0))+\tilde\alpha_1^{-1}g_1'(0)\,,\;\; g_2(0)=-\gamma_2(f_1'(l_1)+f_2'(l_2))+\tilde\alpha_2^{-1}g_2'(0)\,,$$

for some $\alpha_j,\,\tilde\alpha_j,\,\gamma_j\in\mathbb{R}$. Since we want to examine behavior of the model with respect to the lengths of internal edges, let us parametrize them as $l_1=l(1-\lambda)$, $l_2=l(1+\lambda)$ with $\lambda\in[0,1]$; changing λ thus effectively means moving one of the connections points around the loop from the antipolar position for $\lambda=0$ to merging of the two vertices for $\lambda=1$. Due to the presence of the semi-infinite leads the essential (continuous) spectrum of H is $[0,\infty)$. If we consider the loop itself, it has a discrete spectrum consisting of eigenvalues k_n^2 where $k_n=\frac{\pi n}{l}$ with $n\in\mathbb{Z}$. The corresponding eigenfunctions have nodes spaced by $\frac{l}{n}$ for $n\neq 0$, hence H has embedded eigenvalues if the leads are attached to the loop at some of them.

If the rationality of the junction distances is violated these eigenvalues turn into resonances. The condition determining the singularities can be found in the same way as in the previous examples; it reads

$$\sin kl(1-\lambda)\sin kl(1+\lambda)-\frac{4k^2}{\beta_1(k)\beta_2(k)}\sin^2 kl+k\Big[\frac{1}{\beta_1(k)}+\frac{1}{\beta_2(k)}\Big]\sin 2kl=0\,,$$

where $\beta_i^{-1}(k):=\alpha_i^{-1}+\frac{ik|\gamma_i|^2}{1-ik\tilde\alpha_i^{-1}}$. One can solve it perturbatively but also to find numerically its solution describing pole trajectories as λ runs through $[0,1]$. The analysis presented in [EL10] shows that various situations may occur, for instance, a pole returning to the real axis after one or more loops in the complex plane – an example is shown in Figure 3 – or a trajectory ending up in the lower half-plane at the endpoint of the parameter interval.

7.5.2. A cross-shaped graph. We add one more simple example to illustrate that the same effect may occur even if the graph has no loops. Consider a cross-shaped Γ consisting of two leads and two internal edges attached to the leads at one point; the lengths of the internal edges will be $l_1=l(1-\lambda)$ and $l_2=l(1+\lambda)$. The Hamiltonian acts again as $-\mathrm{d}^2/\mathrm{d}x^2$ on the corresponding Hilbert space $L^2(\mathbb{R}^+)\oplus L^2(\mathbb{R}^+)\oplus L^2([0,l_1])\oplus L^2([0,l_2])$ the elements of which are described by columns $\psi=(g_1,g_2,f_1,f_2)^{\mathrm{T}}$. For simplicity we restrict our attention to the δ coupling at the vertex and Dirichlet conditions at the loose ends, i.e., $f_1(0)=f_2(0)=g_1(0)=g_2(0)$ and $f_1(l_1)=f_2(l_2)=0$ together with the requirement

$$f_1'(0)+f_2'(0)+g_1'(0)+g_2'(0)=\alpha f_1(0)$$

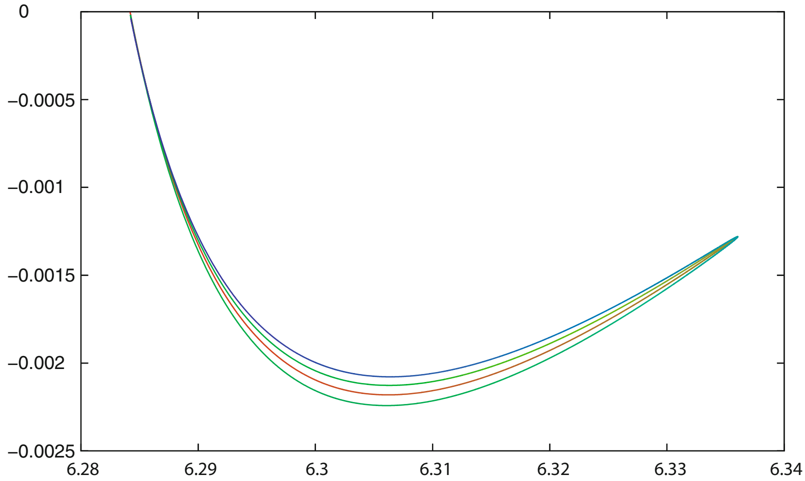

FIGURE 3. Trajectory of the resonance pole in the momentum plane starting from $k_0 = 2\pi$ corresponding to $\lambda = 0$ for $l = 1$ and the coefficients values $\alpha_1^{-1} = 1$, $\tilde{\alpha}_1^{-1} = -2$, $\gamma_1 = 1$, $\alpha_2^{-1} = 0$, $\tilde{\alpha}_2^{-1} = 1$, $\gamma_2 = 1$, $n = 2$.

for $\alpha \in \mathbb{R}$. In the same way as above we can derive resonance condition in the form $k \sin 2kl + (\alpha - 2ik) \sin kl(1-\lambda) \sin kl(1+\lambda) = 0$, or equivalently

$$2k \sin 2kl + (\alpha - 2ik)(\cos 2kl\lambda - \cos 2kl) = 0\,.$$

Asking when the solution is real we note that this happens if the real and imaginary parts of the left-hand side vanish. We find easily that it is the case if $\lambda = 1 - 2m/n$, $\mathbb{N}_0 \ni m \leq n/2$, while if this rationality relation is violated the poles move into the lower half-plane. The condition can be again solved numerically giving pole trajectories for various parameter values; in addition to the possibilities mentioned above we can have trajectories returning to *different* embedded eigenvalues – an example shown in Figure 4 calls to mind the effect of *quantum anholonomy* [Ch98] – as well as avoided trajectory crossings, etc., see [EL10] for more details.

7.5.3. Local multiplicity preservation. Let us turn from examples to the general case and consider an eigenvalue k_0^2 with multiplicity d of a quantum-graph Hamiltonian H which is embedded in the continuous spectrum due to rationality relations between the edges of Γ. We consider graphs Γ_ε with modified edge lengths $l'_j = l_0(n_j + \varepsilon_j)$ assuming that $n_j \in \mathbb{N}$ for $j \in \{1, \dots, n\}$ while n_j may not be an integer for $j \in \{n+1, \dots, N\}$ where $N := \sharp\mathcal{L}$. The analysis of the perturbation is a bit involved, see [EL10] for details, leading to the following conclusion.

Theorem 7.3. *Let Γ be a quantum graph with N finite edges of the lengths l_j, M infinite edges, and the coupling described by the matrix $U = \begin{pmatrix} U_1 & U_2 \\ U_3 & U_4 \end{pmatrix}$, where U_4 corresponds to the coupling between the infinite edges. Let $k_0 > 0$ correspond*

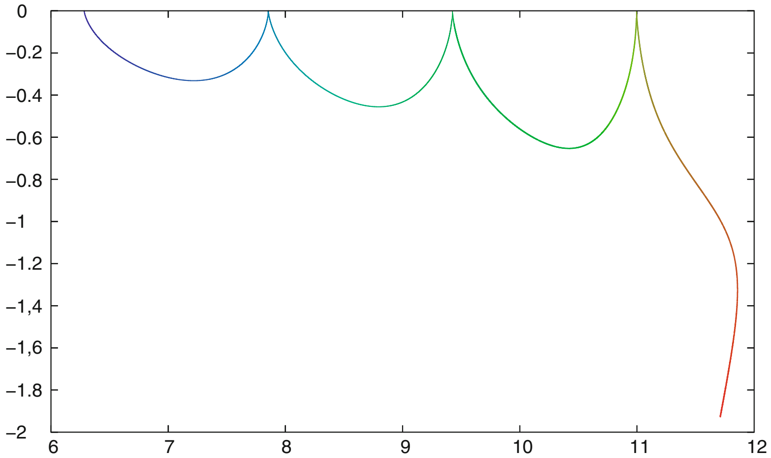

FIGURE 4. Resonance pole trajectory for $\alpha = 1$ and $n = 2$.

to a pole of the resolvent $(H - k_0^2)^{-1}$ of multiplicity d. Let Γ_ε be a geometrically perturbed quantum graph with edge lengths $l_0(n_j + \varepsilon_j)$ described above and the same coupling as Γ. Then there exists an $\varepsilon_0 > 0$ such that for all $\vec{\varepsilon} \in \mathcal{U}_{\varepsilon_0}(0)$ the sum of multiplicities of the resolvent poles in the vicinity of k_0 is d.

8. High-energy behavior of quantum-graph resonances

Now we will look at quantum-graph resonances from a different point of view and ask about asymptotics of their numbers at high energies. Following the papers [DP11, DEL10] we are going to show, in particular, that it may often happen that this asymptotics does not follow the usual Weyl's law. Following the standard convention we will count in this section embedded eigenvalues among resonances speaking about the poles in the open lower half-plane as of 'true' resonances.

8.1. Weyl asymptotics criterion

It is useful for our purpose to rewrite the condition (7.5) in terms of the exponentials e^{ikl_j} and e^{-ikl_j} using for brevity the symbols $e_j^\pm := \mathrm{e}^{\pm ikl_j}$ and $e^\pm := \Pi_{j=1}^N e_j^\pm = e^{\pm ikV}$, where $V = \sum_{j=1}^n l_j$ is the size of the finite part of Γ. The condition then becomes

$$F(k) := \det\left\{\frac{1}{2}[(U-I) + k(U+I)]E_1(k) + \frac{1}{2}[(U-I) - k(U+I)]E_2(k) \right.$$
$$\left. + k(U+I)E_3 + (U-I)E_4 + [(U-I) - k(U+I)]\,\mathrm{diag}\,(0,\dots,0,I_{M\times M})\right\} = 0\,,$$

where $E_i(k) = \text{diag}\left(E_i^{(1)}, E_i^{(2)}, \dots, E_i^{(N)}, 0, \dots, 0\right)$, $i = 1,2,3,4$, are matrices consisting of N nontrivial 2×2 blocks

$$E_1^{(j)} = \begin{pmatrix} 0 & 0 \\ -ie_j^+ & e_j^+ \end{pmatrix},\; E_2^{(j)} = \begin{pmatrix} 0 & 0 \\ ie_j^- & e_j^- \end{pmatrix},\; E_3^{(j)} = \begin{pmatrix} i & 0 \\ 0 & 0 \end{pmatrix},\; E_4^{(j)} = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}.$$

and a trivial $M\times M$ part. To analyze the asymptotics we employ the usual *counting function* $N(R,F)$ defined for an entire function $F(\cdot)$ by

$$N(R,F) = \sharp\{k : F(k) = 0 \text{ and } |k| < R\},$$

where the algebraic multiplicities of the zeros are taken into account. With the above spectral condition in mind we have to apply it to trigonometric polynomials with rational-function coefficients. We need the following result [DEL10] which is a simple consequence of a classical theorem by Langer [La31].

Theorem 8.1. *Let $F(k) = \sum_{r=0}^n a_r(k)\, \mathrm{e}^{ik\sigma_r}$, where $a_r(k)$ are rational functions of the complex variable k with complex coefficients, and $\sigma_r \in \mathbb{R}$, $\sigma_0 < \sigma_1 < \dots < \sigma_n$. Suppose that $\lim_{k\to\infty} a_0(k) \neq 0$ and $\lim_{k\to\infty} a_n(k) \neq 0$. There exists a compact set $\Omega \subset \mathbb{C}$, real numbers m_r and positive K_r, $r = 1,\dots,n$, such that the zeros of $F(k)$ outside Ω lie in one of n logarithmic strips, each one bounded between the curves $-\mathrm{Im}\, k + m_r \log|k| = \pm K_r$. The counting function behaves in the limit $R\to\infty$ as*

$$N(R,F) = \frac{\sigma_n - \sigma_0}{\pi} R + \mathcal{O}(1).$$

To apply this result it is useful to pass to effective energy-dependent coupling (7.6) which makes it possible to cast the spectral condition into a simpler form,

$$F(k) = \det\left\{\frac{1}{2}[(\tilde U(k) - I) + k(\tilde U(k) + I)]\tilde E_1(k) \right. \tag{8.1}$$
$$\left. + \frac{1}{2}[(\tilde U(k) - I) - k(\tilde U(k) + I)]\tilde E_2(k) + k(\tilde U(k) + I)\tilde E_3 + (\tilde U(k) - I)\tilde E_4\right\} = 0,$$

where $\tilde E_j$ are the nontrivial $2N\times 2N$ parts of the matrices E_j, the first two of them being energy-dependent, and I denotes the $2N\times 2N$ unit matrix. Then we have the following criterion [DEL10] for the asymptotics to be of Weyl type.

Theorem 8.2. *Assume a quantum graph (Γ, H_U) corresponding to Γ with finitely many edges and the coupling at vertices $\mathcal{X}_j$ given by unitary matrices U_j. The asymptotics of the resonance counting function as $R\to\infty$ is of the form*

$$N(R,F) = \frac{2W}{\pi} R + \mathcal{O}(1),$$

where the effective size of the graph W satisfies $0 \le W \le V := \sum_{j=1}^N l_j$. Moreover, $W < V$ holds if and only if there exists a vertex where the corresponding energy-dependent coupling matrix $\tilde U_j(k)$ has an eigenvalue $\frac{1-k}{1+k}$ or $\frac{1+k}{1-k}$ for all k.

To prove the theorem one has to realize that $\sigma_n = V$ and $\sigma_0 = -V$, hence the asymptotics is not of Weyl type *iff* either the senior or the junior coefficient in expression of $F(k)$, i.e., those of $e^{\pm}$, vanish. By a straightforward computation [DEL10] we find that they equal $\left(\frac{i}{2}\right)^N \det\left[(\tilde U(k)-I) \pm k(\tilde U(k)+I)\right]$, respectively, and therefore they vanish under the condition stated in the theorem.

Before proceeding further, let us mention that the asymptotic number of resonances is not the only thing of interest. One can investigate other asymptotic properties such as the distribution of resonance pole spacings; quantum graphs are known to be a suitable laboratory to study quantum chaotic effects [KoS03].

8.2. Permutation-symmetric coupling

Let us first look what the above criterion means in a particular class of vertex couplings which are invariant with respect to permutations of the edges connected at the vertex. It is easy to see that such couplings are described by matrices of the form $U_j = a_j J + b_j I$, where a_j, b_j are complex numbers satisfying $|b_j| = 1$ and $|b_j + a_j \deg \mathcal{X}_j| = 1$; the symbol J denotes the square matrix all of whose entries equal to one and I stands for the unit matrix. Important examples are the *δ-coupling* analogous to (7.10), with the functions continuous at the vertex and the sum of outward derivatives proportional to their common value, corresponding to $U_j = \frac{2}{d_j + i\alpha_j} J - I$, where d_j is the number of edges emanating from the vertex $\mathcal{X}_j$ and $\alpha_j \in \mathbb{R}$ is the coupling strength, and the *δ'_{s}-coupling* corresponding to $U_j = -\frac{2}{d_j - i\beta_j} J + I$ with $\beta_j \in \mathbb{R}$ for which the roles of functions and derivatives are interchanged. The particular cases $\alpha_j = 0$ and $\beta_j = 0$ are usually referred to as the Kirchhoff and anti-Kirchhoff condition, respectively.

Consider a vertex which connects p internal and q external edges. For matrices of the form $U_j = a_j J + b_j I$ it is an easy exercise to invert them and to find the effective energy-dependent coupling; this allows us to make the following claim.

Theorem 8.3. *Let (Γ, H_U) be a quantum graph with permutation-symmetric coupling conditions at the vertices, $U_j = a_j J + b_j I$. Then it has a non-Weyl asymptotics if and only if at least one of its vertices is* balanced *in the sense that $p = q$, and the coupling at this vertex satisfies one the following conditions:*

(a) $f_m = f_n, \quad \forall m,n \le 2p, \quad \sum_{m=1}^{2p} f'_m = 0, \quad$ *i.e.*, $U = \frac{1}{p} J_{2p\times 2p} - I_{2p\times 2p}\,,$

(b) $f'_m = f'_n, \quad \forall m,n \le 2p, \quad \sum_{m=1}^{2p} f_j = 0, \quad$ *i.e.*, $U = -\frac{1}{p} J_{2p\times 2p} + I_{2p\times 2p}\,.$

In other words, if the graph has a balanced vertex there are exactly two situations when the asymptotics is non-Weyl, either if the coupling is Kirchhoff – which is the case where the effect was first noted in [DP11] – or if it is anti-Kirchhoff.

8.2.1. An example: a loop with two leads. To illustrate the above claim let us return to the graph of Example 7.5.1. It is balanced if the two leads are attached at the same point. Changing slightly the notation we suppose that the loop length is l and consider the negative Laplacian on the Hilbert space is $L^2(0,l) \oplus L^2(\mathbb{R}^+) \oplus$

$L^2(\mathbb{R}^+)$ with its elements written as $(u, f_1, f_2)^{\mathrm{T}}$ defined on functions from $W^{2,2}_{\mathrm{loc}}(\Gamma)$ satisfying the requirements $u(0) = f_1(0)$ and $u(l) = f_2(0)$ together with

$$\alpha u(0) = u'(0) + f_1'(0) + \beta(-u'(l) + f_2'(0)) \,, \quad \alpha u(l) = \beta(u'(0) + f_1'(0)) - u'(l) + f_2'(0)$$

with real parameters α and β; the choice $\beta = 1$ corresponds to the 'overall' δ-coupling of strength α, while $\beta = 0$ decouples two 'inner-outer' pairs of mutually meeting edges turning Γ into a line with two δ-interactions at the distance l. In terms of the quantities $e^{\pm} = \mathrm{e}^{\pm ikl}$ the pole condition can be written [DEL10] as

$$8\, \frac{i\alpha^2 e^+ + 4k\alpha\beta - i[\alpha(\alpha - 4ik) + 4k^2(\beta^2 - 1)]\, e^-}{4(\beta^2 - 1) + \alpha(\alpha - 4i)} = 0 \,.$$

The coefficient of e^+ vanishes *iff* $\alpha = 0$, the one in the second term for $\beta = 0$ or if $|\beta| \neq 1$ and $\alpha = 0$, while the coefficient e^- does not vanish for any combination of α and β. The graph has thus a non-Weyl asymptotics *iff* $\alpha = 0$. If, in addition, $|\beta| \neq 1$, then all resonances are confined to a circle, i.e., the graph has zero 'effective size'. The only exceptions are the Kirchhoff condition, $\beta = 1$ and $\alpha = 0$, and its anti-Kirchhoff counterpart, $\beta = -1$ and $\alpha = 0$, for which one half of the resonances is asymptotically preserved, in other words, the effective size of the graph is $\frac{1}{2}l$.

We can demonstrate how a 'half' of the resonances disappears using the example of the δ-coupling, $\beta = 1$. The resonance equation in this case becomes

$$\frac{-\alpha \sin kl + 2k(1 + i \sin kl - \cos kl)}{\alpha - 4i} = 0 \,.$$

A simple calculation shows that the graph Hamiltonian has a sequence of embedded eigenvalues k^2 with $k = \frac{2\pi n}{l}$, $n \in \mathbb{Z}$, and a family of resonances given by solutions to $\mathrm{e}^{ikl} = -1 + \frac{4ik}{\alpha}$. The former do not depend on α, while the latter behave like

$$\mathrm{Im}\, k = -\frac{1}{l} \ln \frac{1}{\alpha} + \mathcal{O}(1) \,, \quad \mathrm{Re}\, k = n\pi + \mathcal{O}(\alpha) \,,$$

as $\alpha \to 0$, hence all the 'true' resonances escape to the imaginary infinity in the limit, in analogy with the similar pole behavior described by relation (7.8).

8.3. The mechanism behind a non-Weyl asymptotics

One naturally asks about reasons why graphs with balanced vertices and Kirchhoff/anti-Kirchhoff coupling have smaller than expected effective size. A simple observation is that if such a vertex has degree one, then Kirchhoff coupling between an external and internal edge is in fact no coupling at all, hence the internal edge can be regarded as a part of the lead and the effective size is diminished by its length. We are going to show that this remains true in a sense also when the degree is larger than one.

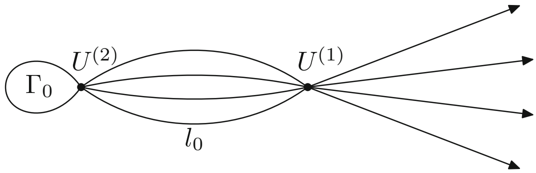

FIGURE 5. Graph with a balanced vertex.

8.3.1. Kirchhoff 'size reduction'. A graph with a balanced vertex can be always thought as having the shape sketched in Figure 5: with a vertex $\mathcal{X}_1$ which connects p internal edges of the same length l_0 and p external edges; if the internal ones have different lengths we simply add a needed number of 'dummy' vertices. We will suppose that the coupling at $\mathcal{X}_1$ is invariant with respect to edge permutations being described by a unitary matrix $U^{(1)} = aJ_{2p\times 2p} + bI_{2p\times 2p}$; the coupling of the other internal edge ends to the rest of the graph, denoted here as Γ_0, is described by a $q \times q$ matrix $U^{(2)}$, where $q \geq p$ (which may express also the topology of Γ_0).

To find how the effective size of such a quantum graph may look like we employ the following property which can be derived easily from coupling condition (7.2).

Proposition 8.4. *Let Γ be the graph described above with the coupling given by arbitrary $U^{(1)}$ and $U^{(2)}$. Let further V be an arbitrary unitary $p\times p$ matrix, $V^{(1)} :=$ diag (V, V) and $V^{(2)} :=$ diag $(I_{(q-p)\times(q-p)}, V)$ be $2p \times 2p$ and $q \times q$ block diagonal matrices, respectively. Then H on Γ is unitarily equivalent to the Hamiltonian H_V on the graph with the same topology and the coupling given by the matrices $[V^{(1)}]^{-1}U^{(1)}V^{(1)}$ and $[V^{(2)}]^{-1}U^{(2)}V^{(2)}$, respectively.*

Application to the couplings described by $U^{(1)} = aJ_{2p\times 2p} + bI_{2p\times 2p}$ at $\mathcal{X}_1$ is straightforward. One has to choose the columns of V as an orthonormal set of eigenvectors of the corresponding $p\times p$ block $aJ_{p\times p}+bI_{p\times p}$ of $U^{(1)}$, the first one of them being $\frac{1}{\sqrt{p}}(1, 1, \dots, 1)^{\mathrm{T}}$. The transformed matrix $[V^{(1)}]^{-1}U^{(1)}V^{(1)}$ decouples then into blocks connecting only the pairs (v_j, g_j). The first one of these, corresponding to a symmetrization of all the u_j's and f_j's, leads to the 2×2 matrix $U_{2\times 2} = apJ_{2\times 2} + bI_{2\times 2}$, while the other lead to separation of the corresponding internal and external edges described by Robin conditions $(b-1)v_j(0) + i(b+1)v_j'(0) = 0$ and $(b-1)g_j(0) + i(b+1)g_j'(0) = 0$ for $j = 2, \dots, p$. We note that it resembles the reduction procedure of a tree graph due to Solomyak [SS02].

It is easy to see that the 'overall' Kirchhoff/anti-Kirchhoff condition at $\mathcal{X}_1$ is transformed to the 'line' Kirchhoff/anti-Kirchhoff condition in the subspace of permutation-symmetric functions, leading to reduction of the graph effective size as mentioned above. In all the other cases the point interaction corresponding to the matrix $apJ_{2\times 2} + bI_{2\times 2}$ is nontrivial, and consequently, the graph size is preserved.

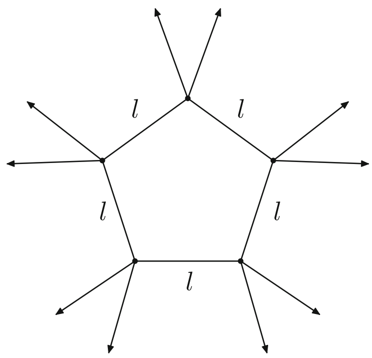

FIGURE 6. A polygonal balanced graph.

8.3.2. Global character of non-Weyl asymptotics. The above reasoning might lead one to the conclusion that the effect discussed here is of a local character. We want to show now that while this is true concerning the occurrence of non-Weyl asymptotics, the effective size of a non-Weyl quantum graph is a global property because it may depend on the graph Γ as a whole.

We will use an example to justify this claim. We shall consider the graph Γ_n with an integer $n \geq 3$ which contains a regular n-gon, each edge of which has length l. To each of its vertices two semi-infinite leads are attached, cf. Figure 6. Hence all the vertices of Γ_n are balanced, and if the coupling in them is of Kirchhoff type the effective size W_n of the graph is by Theorem 8.3 strictly less than the actual size $V_n = n\ell$. It appears, however, that the actual value of the effective size depends in this case on the number n of polygon vertices.

Since all the internal edges have the same length, the system has a rotational symmetry. One can thus perform a 'discrete Floquet' analysis and investigate cells consisting of two internal and two external edges; the wave functions at the ends of the former have to differ by a multiplicative factor ω such that $\omega^n = 1$. After a simple computation [DEL10] we conclude that there is a resonance at k^2 *iff*

$$-2(\omega^2 + 1) + 4\omega e^{-ik\ell} = 0. \tag{8.2}$$

The 'Floquet component' H_ω of H has thus effective size $W_\omega = \frac{1}{2}l$ if $\omega^2 + 1 \neq 0$ while for $\omega^2 + 1 = 0$ we have no resonances, $W_\omega = 0$. Summing finally over all the ω with $\omega^n = 1$ we arrive at the following conclusion.

Theorem 8.5. *The effective size of the graph* Γ_n *with Kirchhoff coupling is*

$$W_n = \begin{cases} \frac{1}{2}nl & \text{if } n \neq 0 \mod 4 \\ \frac{1}{2}(n-2)l & \text{if } n = 0 \mod 4 \end{cases}$$

Note that if one puts $\omega = e^{i\theta}$ in (8.2) the resonance poles behave according to

$$k = \frac{1}{l}\Big(i\ln(\cos\theta) + 2\pi n\Big)$$

where $n \in \mathbb{Z}$ is arbitrary, hence they escape to imaginary infinity as $\theta \to \pm\frac{1}{2}\pi$. Of course, the Floquet variable is discrete, $\theta = \frac{2\pi j}{n}$, $j = 0, 1, \dots, n-1$, nevertheless, the limit still illustrates the mechanism of the resonance 'disappearance'; it is illustrative to look at the behavior of the solutions for large values of n.

8.4. Non-Weyl graphs with non-balanced vertices

Now we are going to show that there are many more graphs with non-Weyl asymptotics once we abandon the assumption of permutation symmetry of the vertex couplings. For the sake of brevity, we limit ourselves again to a simple example. In order to formulate it, however, we state first a general property of the type of Proposition 8.4 above. Specifically, we will ask what happens if the coupling matrix U of a quantum graph is replaced by $W^{-1}UW$, where W is a block diagonal matrix of the form

$$W = \begin{pmatrix} e^{i\varphi} I_{p\times p} & 0 \\ 0 & W_4 \end{pmatrix}$$

and W_4 is a unitary $q \times q$ matrix. The following claim is obtained easily from (7.2).

Proposition 8.6. *The family of resonances of a quantum-graph Hamiltonian H_U does not change if the original coupling matrix U is replaced by $W^{-1}UW$.*

Let us turn now to the example which concerns the graph investigated in Section 7.3, a line with a stub of length l, this time without a potential. Changing slightly the notation we use the symbols f_j for wave function on the two half-lines and u for the stub. The function from the domain of any Hamiltonian H_U are locally $W^{2,2}$ and satisfy the conditions $u(l) + cu'(l) = 0$ with $c \in \mathbb{R} \cup \{\infty\}$ and

$$(U - I)\,(u(0), f_1(0), f_2(0))^{\mathrm{T}} + i(U + I)\,(u'(0), f_1'(0), f_2'(0))^{\mathrm{T}} = 0\,.$$

We split Γ into two parts in a way different from Section 7.3 choosing the coupling described by $U_0 := \mathrm{diag}\left(\left(\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right), e^{i\psi}\right)$ which gives two half-lines with the conditions $u(l) + cu'(l) = 0$ and $f_2(0) + \cot\frac{\psi}{2}\, f_2'(0) = 0$, respectively, at their endpoints; the first part consists of the half-line number one and the stub joined by Kirchhoff coupling. It is obvious that such a graph has at most two resonances, and thus a non-Weyl asymptotics. We now replace U_0 by $U_W = W^{-1}U_0W$ with

$$W = \begin{pmatrix} 1 & 0 & 0 \\ 0 & re^{i\varphi_1} & \sqrt{1-r^2}\, e^{i\varphi_2} \\ 0 & \sqrt{1-r^2}\, e^{i\varphi_3} & -re^{i(\varphi_2+\varphi_3-\varphi_1)} \end{pmatrix}$$

for some $r \in [0, 1]$ and obtain for every fixed value of ψ and c a three-parameter family of coupling conditions described by the unitary matrix

$$U_W = \begin{pmatrix} 0 & re^{i\varphi_1} & \sqrt{1-r^2} e^{i\varphi_2} \\ re^{-i\varphi_1} & (1-r^2)e^{i\psi} & -r\sqrt{1-r^2} e^{-i(-\psi+\varphi_1-\varphi_2)} \\ \sqrt{1-r^2} e^{-i\varphi_2} & -r\sqrt{1-r^2} e^{i(\psi+\varphi_1-\varphi_2)} & r^2 e^{i\psi} \end{pmatrix},$$

each of which has the same resonances as U_0 by Proposition 8.6. The associated quantum graphs are thus of non-Weyl type despite the fact that their edges are connected in a single vertex of Γ which is not balanced.

Note that among these couplings one can find, in particular, the one mentioned above in connection with relation (7.8); choosing $\psi = \pi$ and $c = 0$, and furthermore, $\varphi_1 = \varphi_2 = 0$ and $r = 2^{-1/2}$, we get the conditions

$$f_1(0) = f_2(0), \quad u(0) = \sqrt{2} f_1(0), \quad f_1'(0) - f_2'(0) = -\sqrt{2} u'(0)\,,$$

or (7.7) with $b = \sqrt{2}$ and $c = d = 0$. Similarly, such conditions with $b = -\sqrt{2}$ and $c = d = 0$ correspond to $\varphi_1 = \varphi_2 = \pi$ and $r = 2^{-1/2}$; both these quantum graphs have no resonances at all. This fact is easily understandable, for instance, if we regard the line with the stub as a tree with the root at the end of the stub and apply the Solomyak reduction procedure [SS02] mentioned above.

8.5. Magnetic field influence

Let us finally look how can the high-energy asymptotics be influenced by a magnetic field. We have encountered magnetic quantum graphs already in the example of Section 7.4, now we look at them in more generality. We consider a graph Γ with a set of vertices $\{\mathcal{X}_j\}$ and set of edges $\{\mathcal{E}_j\}$ containing N finite edges and M infinite leads. We assume that it is equipped with the operator H acting as $-\frac{\mathrm{d}^2}{\mathrm{d}x^2}$ on the infinite leads and as $-(\frac{\mathrm{d}}{\mathrm{d}x} + iA_j(x))^2$ on the internal edges, where A_j is the tangent component of the vector potential; without loss of generality we may neglect it on external leads because one can always remove it there by a gauge transformation. The Hamiltonian domain consists of functions from $W^{2,2}_{\mathrm{loc}}(\Gamma)$ which satisfy $(U_j - I)\Psi_j + i(U_j + I)(\Psi_j' + i\mathcal{A}_j\Psi_j) = 0$ at the vertex $\mathcal{X}_j$. As before it is useful to pass to a graph Γ_0 with a single vertex of degree $(2N + M)$ in which the coupling is described by the condition

$$(U - I)\Psi + i(U + I)(\Psi' + i\mathcal{A}\Psi) = 0\,,$$

where the matrix U consists of the blocks U_j corresponding to the vertices of Γ and the matrix $\mathcal{A}$ is composed of tangent components of the vector potential at the vertices, $\mathcal{A} = \mathrm{diag}\,(A_1(0), -A_1(l_1), \dots, A_N(0), -A_N(l_N), 0, \dots, 0)$.

Using the local gauge transformation $\psi_j(x) \mapsto \psi_j(x)\mathrm{e}^{-i\chi_j(x)}$ with $\chi_j(x)' = A_j(x)$ one can get rid of the explicit dependence of coupling conditions on the magnetic field and arrive thus at the Hamiltonian acting as $-\frac{\mathrm{d}^2}{\mathrm{d}x^2}$ with the coupling conditions given by a transformed unitary matrix,

$$(U_A - I)\Psi + i(U_A + I)\Psi' = 0\,, \quad U_A := \mathcal{F}U\mathcal{F}^{-1}, \tag{8.3}$$

with $\mathcal{F} = \mathrm{diag}\,(1, \exp(i\Phi_1), \dots, 1, \exp(i\Phi_N), 1, \dots, 1)$ containing magnetic fluxes $\Phi_j = \int_0^{l_j} A_j(x)\,\mathrm{d}x$. Furthermore, one can reduce the analysis to investigation of the compact core of Γ with an effective energy-dependent coupling described by the matrix $\tilde{U}_A(k)$ obtained from U_A in analogy with (7.5).

To answer the question mentioned above we employ another property of the type of Proposition 8.4. This time we consider replacement of U by $V^{-1}UV$ where $V = \begin{pmatrix} V_1 & 0 \\ 0 & V_2 \end{pmatrix}$ is unitary block-diagonal matrix consisting of a $2N \times 2N$ block V_1 and an $M \times M$ block V_2; resonances are again invariant under this transformation. With respect to the relation between U and $\tilde{U}_A$ we get the following result [EL11].

Theorem 8.7. *A quantum graph with a magnetic field described by a vector potential A is of non-Weyl type if and only if the same is true for $A = 0$.*

In other words, magnetic field alone cannot switch a graph with non-Weyl asymptotics into Weyl type and *vice versa*. On the other hand, the magnetic field *can* change the effective size of a non-Weyl graph. To illustrate this claim, let us return to the example discussed in Section 7.5.1, a loop with two external leads Kirchhoff-coupled to a single point, now we add a magnetic field. It is straightforward to check [EL11] that the condition determining the resonance pole becomes

$$-2\cos\Phi + \mathrm{e}^{-ikl} = 0\,,$$

where Φ is the magnetic flux through the loop. The graph is non-Weyl as the term with e^{ikl} is missing on the left-hand side; if $\Phi = \pm\pi/2 \pmod{\pi}$, that is, for odd multiples of a quarter of the flux quantum 2π, the l-independent term disappears and the effective size of the graph becomes zero.

The conclusions of the example can be generalized [EL11] to any graph with a single internal edge: if the elements of the effective 2×2 coupling matrix satisfy $|\tilde{u}_{12}(k)| = |\tilde{u}_{21}(k)|$ for any $k > 0$ there is a magnetic field such that the graph under its influence has at most finite number of resonances.

9. Leaky graphs: a caricature of quantum wires and dots

A different class of quantum graph models employs Schrödinger operators which can be formally written as $-\Delta - \alpha\delta(x-\Gamma)$ where $\Gamma \subset \mathbb{R}^d$ is a graph; one usually speaks about *'leaky' graphs*. Their advantage is that they can take into account tunneling between different parts of the graph as well as its geometry beyond just the edge lengths. A survey of results concerning these models can be found in [Ex08]. In particular, even a simple Γ like an infinite non-straight curve can give rise to resonances [EN03], however, one needs a numerical analysis to reveal them.

9.1. The model

Instead we will describe here a simple model of this type which can be regarded as a caricature description of a system consisting of a quantum wire and one or several quantum dots. The state Hilbert space of the model is $L^2(\mathbb{R}^2)$ and the Hamiltonian can be formally written as

$$-\Delta - \alpha\delta(x-\Sigma) + \sum_{i=1}^{n} \tilde{\beta}_i \delta(x - y^{(i)})\,,$$

where $\alpha > 0$, $\Sigma := \{(x_1, 0);\, x_1 \in \mathbb{R}\}$, and $\Pi := \{y^{(i)}\}_{i=1}^n \subset \mathbb{R}^2 \setminus \Sigma$. The formal coupling constants of the two-dimensional δ potentials are marked by tildes to stress they are not identical with the proper coupling parameters β_i which we shall introduce below. Following the standard prescription [AGHH] one can define the operator rigorously [EK04] by introducing appropriated boundary conditions on $\Sigma\cup\Pi$. Consider functions $\psi \in W^{2,2}_{\mathrm{loc}}(\mathbb{R}^2\setminus(\Sigma\cup\Pi))\cap L^2$ continuous on Σ. For a small enough $\rho > 0$ the restriction $\psi\restriction_{\mathcal{C}_{\rho,i}}$ to the circle $\mathcal{C}_{\rho,i} := \{q \in \mathbb{R}^2 : |q - y^{(i)}| = \rho\}$ is well defined; we say that ψ belongs to $D(\dot{H}_{\alpha,\beta})$ *iff* $(\partial_{x_1}^2 + \partial_{x_2}^2)\psi$ on $\mathbb{R}^2 \setminus (\Sigma \cup \Pi)$ belongs to L^2 in the sense of distributions and the limits

$$\Xi_i(\psi) := -\lim_{\rho\to 0} \frac{1}{\ln\rho}\,\psi\restriction_{\mathcal{C}_{\rho,i}}, \;\; \Omega_i(\psi) := \lim_{\rho\to 0}[\psi\restriction_{\mathcal{C}_{\rho,i}} + \Xi_i(\psi)\ln\rho]\,, \;\; i = 1,\dots,n\,,$$

$$\Xi_\Sigma(\psi)(x_1) := \partial_{x_2}\psi(x_1,0+) - \partial_{x_2}\psi(x_1,0-)\,, \quad \Omega_\Sigma(\psi)(x_1) := \psi(x_1,0)$$

exist, they are finite, and satisfy the relations

$$2\pi\beta_i\Xi_i(\psi) = \Omega_i(\psi)\,, \quad \Xi_\Sigma(\psi)(x_1) = -\alpha\Omega_\Sigma(\psi)(x_1)\,, \tag{9.1}$$

where $\beta_i \in \mathbb{R}$ are the true coupling parameters; we put $\beta = (\beta_1,\dots,\beta_n)$ in the following. On this domain we define the operator $\dot{H}_{\alpha,\beta} : D(\dot{H}_{\alpha,\beta}) \to L^2(\mathbb{R}^2)$ by

$$\dot{H}_{\alpha,\beta}\psi(x) = -\Delta\psi(x) \quad \text{for} \quad x \in \mathbb{R}^2 \setminus (\Sigma \cup \Pi)\,.$$

It is now a standard thing to check that $\dot{H}_{\alpha,\beta}$ is essentially self-adjoint [EK04]; we shall regard in the following its closure denoted as $H_{\alpha,\beta}$ as the rigorous counterpart to the above-mentioned formal model Hamiltonian.

To find the resolvent of $H_{\alpha,\beta}$ we start from $R(z) = (-\Delta - z)^{-1}$ which is for any $z \in \mathbb{C}\setminus[0,\infty)$ an integral operator with the kernel $G_z(x,x') = \frac{1}{2\pi}K_0(\sqrt{-z}|x-x'|)$, where K_0 is the Macdonald function and $z \mapsto \sqrt{z}$ has conventionally a cut along the positive half-line; we denote by $\mathbf{R}(z)$ the unitary operator with the same kernel acting from $L^2(\mathbb{R}^2)$ to $W^{2,2}(\mathbb{R}^2)$. We need two auxiliary spaces, $\mathcal{H}_0 := L^2(\mathbb{R})$ and $\mathcal{H}_1 := \mathbb{C}^n$, and the corresponding trace maps $\tau_j : W^{2,2}(\mathbb{R}^2) \to \mathcal{H}_j$ which act as

$$\tau_0\psi := \psi\restriction_\Sigma\,, \quad \tau_1\psi := \psi\restriction_\Pi = \left(\psi\restriction_{\{y^{(1)}\}},\dots,\psi\restriction_{\{y^{(n)}\}}\right),$$

respectively; they allow us to define the canonical embeddings of $\mathbf{R}(z)$ to $\mathcal{H}_i$, i.e.,

$$\mathbf{R}_{iL}(z) = \tau_i R(z) : L^2 \to \mathcal{H}_i\,, \quad \mathbf{R}_{Li}(z) = [\mathbf{R}_{iL}(z)]^* : \mathcal{H}_i \to L^2\,,$$

and $\mathbf{R}_{ji}(z) = \tau_j\mathbf{R}_{Li}(z) : \mathcal{H}_i \to \mathcal{H}_j$, all expressed naturally through the free Green's function in their kernels, with the variable range corresponding to a given $\mathcal{H}_i$. The operator-valued matrix $\Gamma(z) = [\Gamma_{ij}(z)] : \mathcal{H}_0 \oplus \mathcal{H}_1 \to \mathcal{H}_0 \oplus \mathcal{H}_1$ is defined by

$$\begin{aligned} \Gamma_{ij}(z)g &:= -\mathbf{R}_{ij}(z)g \qquad \text{for} \quad i \neq j \quad \text{and} \quad g \in \mathcal{H}_j\,, \\ \Gamma_{00}(z)f &:= \left[\alpha^{-1} - \mathbf{R}_{00}(z)\right]f \qquad \text{if} \;\; f \in \mathcal{H}_0\,, \\ \Gamma_{11}(z)\varphi &:= \left[s_{\beta_l}(z)\delta_{kl} - G_z(y^{(k)},y^{(l)})(1-\delta_{kl})\right]_{k,l=1}^n \varphi \quad \text{for} \;\; \varphi \in \mathcal{H}_1\,, \end{aligned}$$

where $s_{\beta_l}(z) = \beta_l + s(z) := \beta_l + \frac{1}{2\pi}(\ln\frac{\sqrt{z}}{2i} - \psi(1))$ and $-\psi(1)$ is the Euler number. For z from $\rho(H_{\alpha,\beta})$ the operator $\Gamma(z)$ is boundedly invertible. In particular, $\Gamma_{00}(z)$ is invertible which makes it possible to employ the Schur reduction procedure one more time and to define the map $D(z) : \mathcal{H}_1 \to \mathcal{H}_1$ by

$$D(z) = \Gamma_{11}(z) - \Gamma_{10}(z)\Gamma_{00}(z)^{-1}\Gamma_{01}(z)\,. \tag{9.2}$$

We call it the *reduced determinant* of Γ; it allows us to write the inverse of $\Gamma(z)$ as $[\Gamma(z)]^{-1} : \mathcal{H}_0 \oplus \mathcal{H}_1 \to \mathcal{H}_0 \oplus \mathcal{H}_1$ with the 'block elements' defined by

$$\begin{aligned}
[\Gamma(z)]_{11}^{-1} &= D(z)^{-1}\,,\\
[\Gamma(z)]_{00}^{-1} &= \Gamma_{00}(z)^{-1} + \Gamma_{00}(z)^{-1}\Gamma_{01}(z)D(z)^{-1}\Gamma_{10}(z)\Gamma_{00}(z)^{-1}\,,\\
[\Gamma(z)]_{01}^{-1} &= -\Gamma_{00}(z)^{-1}\Gamma_{01}(z)D(z)^{-1}\,,\\
[\Gamma(z)]_{10}^{-1} &= -D(z)^{-1}\Gamma_{10}(z)\Gamma_{00}(z)^{-1}\,;
\end{aligned}$$

in the above formulae we use the notation $\Gamma_{ij}(z)^{-1}$ for the inverse of $\Gamma_{ij}(z)$ and $[\Gamma(z)]_{ij}^{-1}$ for the matrix elements of $[\Gamma(z)]^{-1}$.

Before using this to express the resolvent $R_{\alpha,\beta}(z) := (H_{\alpha,\beta} - z)^{-1}$ we introduce another notation which allow us to write $R_{\alpha,\beta}(z)$ through a perturbation of the 'line only' Hamiltonian $\tilde{H}_\alpha$ describing the system without the point interactions, i.e., $\beta_i = \infty$, $i = 1, \dots, n$. By [BEKŠ94] the resolvent of $\tilde{H}_\alpha$ is equal to

$$R_\alpha(z) = R(z) + R_{L0}(z)\Gamma_{00}^{-1}R_{0L}(z)$$

for $z \in \mathbb{C} \setminus [-\frac{1}{4}\alpha^2, \infty)$. We define the map $\mathbf{R}_{\alpha;L1}(z) : \mathcal{H}_1 \to L^2(\mathbb{R}^2)$ by $\mathbf{R}_{\alpha;1L}(z)\psi := R_\alpha(z)\psi \upharpoonright_\Pi$ and $\mathbf{R}_{\alpha;1L}(z) : L^2(\mathbb{R}^2) \to \mathcal{H}_1$ as its adjoint, $\mathbf{R}_{\alpha;L1}(z) := \mathbf{R}^*_{\alpha;1L}(z)$. The resolvent difference between $H_{\alpha,\beta}$ and $\tilde{H}_\alpha$ is then given by Krein's formula [AGHH]. A straightforward computation [EK04] yields now the following result.

Theorem 9.1. *For any* $z \in \rho(H_{\alpha,\beta})$ *with* $\operatorname{Im} z > 0$ *we have*

$$R_{\alpha,\beta}(z) = R(z) + \sum_{i,j=0}^{1} \mathbf{R}_{Li}(z)[\Gamma(z)]_{ij}^{-1}\mathbf{R}_{jL}(z) = R_\alpha(z) + \mathbf{R}_{\alpha;L1}(z)D(z)^{-1}\mathbf{R}_{\alpha;1L}(z)\,.$$

The obtained resolvent expressions allow us to investigate various spectral properties of the operator $H_{\alpha,\beta}$ [EK04]; here we concentrate only on those related to the subject of the paper, namely to perturbations of embedded eigenvalues.

9.2. Resonance poles

The mechanism governing resonance and decay phenomena in this model is the tunneling between the points and the line. This interaction can be 'switched off' if the line is removed, in other words, put to infinite distance from the points. Consequently, the 'free' Hamiltonian $\tilde{H}_\beta := H_{0,\beta}$ has the point interactions only. It has m eigenvalues, $1 \le m \le n$ of which we assume

$$-\frac{1}{4}\alpha^2 < \epsilon_1 < \cdots < \epsilon_m < 0\,, \tag{9.3}$$

i.e., that the discrete spectrum of $\tilde{H}_\beta$ is simple and contained in (the negative part of) $\sigma(\tilde{H}_\alpha) = \sigma_{ac}(H_{\alpha,\beta}) = [-\frac{1}{4}\alpha^2, \infty)$; this can be always achieved by an appropriate choice of the configuration of the set Π and the coupling parameters β. Let us specify the interactions sites by their Cartesian coordinates, $y^{(i)} = (c_i, a_i)$. It is also useful to introduce the notations $a = (a_1, \dots, a_n)$ and $d_{ij} = |y^{(i)} - y^{(j)}|$ for the distances between the point interactions.

Resolvent poles will be found through zeros of the operator-valued function (9.2), more exactly, through the analytical continuation of $D(\cdot)$ to a subset Ω_- of the lower half-plane across the segment $(-\frac{1}{4}\alpha^2, 0)$ of the real axis, in a similar way to what we did for Friedrichs model using formula (3.3). For the sake of definiteness we employ the notation $D(\cdot)^{(l)}$, where $l = -1, 0, 1$ refers to the argument z from Ω_-, the segment $(-\frac{1}{4}\alpha^2, 0)$, and the upper half-plane, $\mathrm{Im}\, z > 0$, respectively. Using the resolvent formula of the previous section we see that the first component of the operator-valued function $D(\cdot)^{(l)}$ is an $n \times n$ matrix with the elements

$$\Gamma_{11;jk}(z)^{(l)} = -(1-\delta_{jk})\,\frac{1}{2\pi} K_0\big(d_{jk}\sqrt{-z}\big) + \delta_{jk}\big(\beta_j + 1/2\pi(\ln\sqrt{-z} - \psi(1))\big)$$

for all the l. To find an explicit form of the second component let us introduce

$$\mu_{ij}(z,t) := \frac{i\alpha}{2^5\pi}\,\frac{(\alpha - 2i(z-t)^{1/2})\,\mathrm{e}^{i(z-t)^{1/2}(|a_i|+|a_j|)}}{t^{1/2}(z-t)^{1/2}}\,\mathrm{e}^{it^{1/2}(c_i-c_j)}$$

and $\mu^0_{ij}(\lambda,t) := \lim_{\eta\to 0+}\mu_{ij}(\lambda + i\eta, t)$. Using this notation we can rewrite the matrix elements of $(\Gamma_{10}\Gamma_{00}^{-1}\Gamma_{01})^{(l)}(z)$ appearing in (9.2) in the following form,

$$\theta^{(0)}_{ij}(\lambda) = \mathcal{P}\int_0^\infty \frac{\mu^0_{ij}(\lambda,t)}{t-\lambda-\frac{1}{4}\alpha^2}\,\mathrm{d}t + g_{\alpha,ij}(\lambda)\,, \qquad \lambda \in \big(-\tfrac{1}{4}\alpha^2, 0\big)$$

$$\theta^{(l)}_{ij}(z) = l\int_0^\infty \frac{\mu_{ij}(z,t)}{t-z-\frac{1}{4}\alpha^2}\,\mathrm{d}t + (l-1)g_{\alpha,ij}(z) \quad \text{for } \ l = 1,\,-1$$

where $\mathcal{P}$ indicates again principal value of the integral, and

$$g_{\alpha,ij}(z) := \frac{i\alpha}{(z+\alpha^2/4)^{1/2}}\,\mathrm{e}^{-\alpha(|a_i|+|a_j|)/2}\,\mathrm{e}^{i(z+\alpha^2/4)^{1/2}(c_i-c_j)}\,.$$

Using these formulae one has to find zeros of $\det D(\cdot)^{(-1)}$; we shall sketch the argument referring to [EK04, EIK07] for details. We have mentioned that resonances are caused by tunneling between the parts of the interaction support, hence it is convenient to introduce the following reparametrization,

$$b(a) = (b_1(a), \dots, b_n(a)) \quad \text{with} \quad b_i(a) := \mathrm{e}^{-|a_i|\sqrt{-\epsilon_i}}$$

and to put $\eta(b(a), z) := \det D(z)^{(-1)}$. Since the absence of the line-supported interaction can be regarded as putting the line to an infinite distance from the points, it corresponds to $b = 0$ in which case we have $\eta(0,z) = \det\Gamma_{11}(z)$ and the zeros are nothing else than the eigenvalues of the point-interaction Hamiltonian $\tilde{H}_\beta$, in other words, $\eta(0,\epsilon_i) = 0\,,\ i = 1,\dots,m$. Then, in analogy with Sec. 3, we have to check that the hypotheses of the implicit-function theorem are satisfied which makes it possible to formulate the following conclusion.

Proposition 9.2. *The equation $\eta(b,z) = 0$ has for all the b_i small enough exactly m zeros which admit the following weak-coupling asymptotic expansion,*

$$z_i(b) = \epsilon_i + \mathcal{O}(|b|) + i\mathcal{O}(|b|) \quad \text{where} \quad |b| := \max_{1\le i\le m} b_i\,.$$

This result is not very strong, because it does provides just a bound on the asymptotic behavior and it does not guarantee that the interaction turns embedded eigenvalues of $\tilde{H}_\beta$ into true resonances. This can be checked in the case $n = 1$ [EK04] but it may not be true already for $n = 2$. The simplest example involves a pair of point interactions with the same coupling placed in a mirror-symmetric way with respect to Σ. The Hamiltonian can then be decomposed according to parity, its part acting on functions even with respect to Σ has a resonance, exponentially narrow in terms of the distance between the points and the line, while the odd one has a embedded eigenvalue independently of the distance. On the other hand, if the mirror symmetry is violated, be it by changing one of the point distances or one of the coupling constants, the latter turns into a resonance and one can derive a weak-perturbation expansion [EK04] in a way similar to those of Section 4.1.

Let us also note that the explicit form of the resolvent given in Theorem 9.1 makes it possible to find the on-shell S-matrix from energies from the interval $(-\frac{1}{4}\alpha^2, 0)$, that is, for states travelling along the 'wire', and to show that their poles coincide with the resolvent poles; for $m = 1$ this is done in [EK04].

9.3. Decay of the 'dot' states

The present model gives us one more opportunity to illustrate relations between resonances and time evolution of unstable systems, this time on bound states of the quantum 'dots' decaying due to tunneling between them and the 'wire'. By assumption (9.3) there is a nontrivial discrete spectrum of $\tilde{H}_\beta$ embedded in $(-\frac{1}{4}\alpha^2, 0)$, and the respective eigenfunctions are

$$\psi_j(x) = \sum_{i=1}^{m} d_i^{(j)} \phi_i^{(j)}(x)\,,\; j = 1, \dots, m\,, \quad \phi_i^{(j)}(x) := \sqrt{-\frac{\epsilon_j}{\pi}}\, K_0\big(\sqrt{-\epsilon_j}|x - y^{(i)}|\big)\,,$$

where in accordance with [AGHH, Sec. II.3] the coefficient vectors $d^{(j)} \in \mathbb{C}^m$ solve the equation $\Gamma_{11}(\epsilon_j)d^{(j)} = 0$ and the normalization condition $\|\phi_i^{(j)}\| = 1$ gives

$$|d^{(j)}|^2 + 2\mathrm{Re} \sum_{i=2}^{m} \sum_{k=1}^{i-1} \overline{d_i^{(j)}} d_k^{(j)} (\phi_i^{(j)}, \phi_k^{(j)}) = 1\,.$$

In particular, $d^{(1)} = 1$ if $n = m = 1$; if $m > 1$ and the distances between the points of Π are large, the natural length scale being given by $(-\epsilon_j)^{-1/2}$, the cross terms are small and the vector lengths $|d^{(j)}|$ are close to one.

Let us now identify the unstable system Hilbert space $\mathcal{H}_\mathrm{u} = E_\mathrm{u} L^2(\mathbb{R}^2)$ with the span of the vectors $\psi_1, \dots, \psi_m$. The decay law of the system prepared at the initial instant $t = 0$ at a state $\psi \in \mathcal{H}_\mathrm{u}$ is according to (2.1) given by the formula

$$P_\psi(t) = \|E_\mathrm{u}\, \mathrm{e}^{-iH_{\alpha,\beta}t}\psi\|^2.$$

We are particularly interested in the *weak-coupling situation* which in the present case means that the distance between Σ and Π is a large at the scale given by $(-\epsilon_m)^{-1/2}$. Let us denote by E_j the one-dimensional projection associated with the eigenfunction ψ_j, the one can make the following claim [EIK07].

Theorem 9.3. *Suppose that $H_{\alpha,\beta}$ has no embedded eigenvalues. Then, with the notation introduced above, we have in the limit $|b| \to 0$, i.e.,* $\mathrm{dist}\,(\Sigma, \Pi) \to \infty$

$$\|E_j\, \mathrm{e}^{-iH_{\alpha,\beta}t}\psi_j - \mathrm{e}^{-iz_j t}\psi_j\| \to 0\,,$$

pointwise in $t \in (0, \infty)$, which for $n = 1$ implies $|P_{\psi_1}(t) - \mathrm{e}^{2\mathrm{Im}\, z_1 t}| \to 0$ as $|b| \to 0$.

Let us add a couple of remarks. The result implies more generally that for large values of $\mathrm{dist}\,(\Sigma, \Pi)$ the reduced evolution can be approximated by a semi-group. On the other hand, despite the approximately exponential decay in the case $n = 1$ the lifetime defined as $T_{\psi_1} = \int_0^\infty P_{\psi_1}(t)\, \mathrm{d}t$ diverges; the situation is similar to those mentioned is Sections 3 and 5.1: the operator $H_{\alpha,\beta}$ has a bound state which is not exactly orthogonal to ψ_1 for $b \neq 0$, cf. [EK04], hence $\lim_{t\to\infty} P_{\psi_1}(t) \neq 0$. Furthermore, the decay of the 'dot' states in this model offers a possibility to compare the 'stable' dynamics, i.e., evolution of vector in $\mathcal{H}_\mathrm{u}$ governed $\mathrm{e}^{-i\tilde{H}_\beta t}$, with the Zeno dynamics obtained from $\mathrm{e}^{-iH_{\alpha,\beta}t}$ by permanent observation. cf. [EIK07] for details. Finally, let us finally mention that a related model with a singular interaction in $\mathbb{R}^3$ supported by a line and a circle and resonances coming from a symmetry violation has been investigated recently in [Ko12].

10. Generalized graphs

In the closing section we will mention another class of solvable models in which resonances can be studied, which may be regarded as another generalization of the quantum graphs discussed in Section 7. What they have in common is that the configuration space consists of parts connected together through point contacts. In the present case, however, we consider parts of different dimensions; for simplicity we limit ourselves to the simplest situation when the dimensions are one and two.

10.1. Coupling different dimensions

To begin with we have to explain how such a coupling can be constructed. The technique is known since [EŠ87], we demonstrate it on the simplest example in which a half-line lead is coupled to a plane. In this case the state Hilbert space is $L^2(\mathbb{R}^-) \oplus L^2(\mathbb{R}^2)$ and the Hamiltonian acts on its elements $\binom{\psi_\mathrm{lead}}{\psi_\mathrm{plane}}$ (belonging locally to $W^{2,2}$) as $\binom{-\psi''_\mathrm{lead}}{-\Delta\psi_\mathrm{plane}}$; to make such an operator self-adjoint one has to impose suitable boundary conditions which couple the wave functions at the junction.

The boundary values to enter such boundary condition are obvious on the lead side being the columns of the values $\psi_\mathrm{lead}(0+)$ and $\psi'_\mathrm{lead}(0+)$. On the other hand, in the plane we have to use generalized ones analogous to those appearing in the first relation of (9.1). If we restrict the two-dimensional Laplacian to functions vanishing at the origin and take an adjoint to such an operator, the functions in the corresponding domain will have a logarithmic singularity at the origin and the generalized boundary values will be the coefficients in the corresponding expansion,

$$\psi_{\mathrm{plane}}(x) = -\frac{1}{2\pi}\, L_0(\psi_{\mathrm{plane}})\, \ln|x| + L_1(\psi_{\mathrm{plane}}) + o(|x|)\,;$$

using them we can write the sought coupling conditions as

$$\begin{aligned} \psi'_{\mathrm{lead}}(0+) &= A\psi_{\mathrm{lead}}(0+) + 2\pi\bar{C}L_0(\psi_{\mathrm{plane}})\,, \\ L_1(\psi_{\mathrm{plane}}) &= C\psi_{\mathrm{lead}}(0+) + DL_0(\psi_{\mathrm{plane}})\,, \end{aligned} \tag{10.1}$$

where $A, D \in \mathbb{R}$ and C is a complex number, or more generally

$$\mathcal{A}\begin{pmatrix} \psi_{\mathrm{lead}}(0+) \\ L_0(\psi_{\mathrm{plane}}) \end{pmatrix} + \mathcal{B}\begin{pmatrix} \psi'_{\mathrm{lead}}(0+) \\ L_1(\psi_{\mathrm{plane}}) \end{pmatrix} = 0$$

with appropriately chosen matrices $\mathcal{A}, \mathcal{B}$ in analogy with (7.2), however, for our purpose here the generic conditions (10.1) are sufficient.

As in the case of quantum graphs the choice of the coupling based on the probability current conservations leaves many possibilities open and the question is which ones are physically plausible. This is in general a difficult problem. A natural strategy would be to consider leads of finite girth coupled to a surface and the limit when the transverse size tends to zero. While for quantum graphs such limits are reasonably well understood nowadays [Gr08, EP09, CET10, EP13], for mixed dimensions the current knowledge is limited to heuristic results such as the one in [EŠ97] which suggests that an appropriate parameter choice in (10.1) might be

$$A = \frac{1}{2\rho}\,, \quad B = \sqrt{\frac{2\pi}{\rho}}\,, \quad C = \frac{1}{\sqrt{2\pi\rho}}\,, \quad D = -\ln\rho\,, \tag{10.2}$$

where ρ is the contact radius. At the same time, other possibilities have been considered such as the simplest choice keeping just the coupling term, $A = D = 0$, or an indirect approach based on fixing the singularity of the Hamiltonian Green's function at the junction which avoids using the coupling conditions explicitly [Ki97].

While the example concerned a particular case, the obtained coupling conditions are of a local character and can be employed whenever we couple a one-dimensional lead to a locally smooth surface. In this way one can treat a wide class of such systems, in particular to formulate the scattering theory on configuration spaces consisting of a finite numbers of manifolds, finite and infinite edges – one sometimes speaks about 'hedgehog manifolds' – cf. [BG03].

Before turning to an example of resonances on such a 'manifold' let us mention that while the system of a plane and a half-line lead considered above has at most two resonances coming from the coupling, one can produce an infinite series of them if the motion in the plane is under influence of a magnetic field. The same is true even if Laplacian is replaced by a more complicated Hamiltonian describing other physical effects such as spin-orbit interaction – cf. [CE11].

10.2. Transport through a geometric scatterer

Let us look in more detail into an important example in which we have a 'geometric scatterer' consisting of a compact and connected manifold Ω, which may or may not have a boundary, to which two semi-infinite leads are attached at two different points x_1, x_2 from the interior of Ω. One may regard such a system as a motion on the line which is cut and the loose ends are attached to a black-box object which can be characterized by the appropriate transfer matrix, $\binom{u(0+)}{u'(0+)} = L\binom{u(0-)}{u'(0-)}$. To find the latter one has to fix the dynamics: we suppose that the motion on the line is free being described by the negative Laplacian, while the manifold part of the Hamiltonian is Laplace–Beltrami operator on the state Hilbert space $L^2(\Omega)$ of the scatterer; they are coupled by conditions (10.1) with the coefficients indexed by $j = 1, 2$ referring to the 'left' and 'right' lead, respectively.

We need the Green function $G(.,.;k)$ of the Laplace–Beltrami operator which exists whenever the k^2 does not belong to the spectrum. Its actual form depends on the geometry of Ω but the diagonal singularity does not: the manifold Ω admits in the vicinity of any point a local Cartesian chart and the Green function behaves with respect to those variables as that of the Laplacian in the plane,

$$G(x,y;k) = -\frac{1}{2\pi}\ln|x-y| + \mathcal{O}(1)\,, \qquad |x-y| \to 0\,.$$

Looking for transient solutions to the Schrödinger equation at energy k^2, we note that its manifold part can be written as $u(x) = a_1 G(x,x_1;k) + a_2 G(x,x_2;k)$, cf. [Ki97], which allows us to find the generalized boundary values

$$L_0(x_j) = -\frac{a_j}{2\pi}\,, \qquad L_1(x_j) = a_j\xi(x_j,k) + a_{3-j}G(x_1,x_2;k)$$

for $j = 1, 2$, where we have employed the regularized Green function at x_j,

$$\xi(x_j;k) := \lim_{x\to x_j}\left[G(x,x_j;k) + \frac{\ln|x-x_j|}{2\pi}\right]. \tag{10.3}$$

Let u_j be the wave function on the jth lead; using the abbreviations u_j, u_j' for its boundary values we get from the conditions (10.1) a linear system which can be easily solved [ETV01]; it yields the transfer matrix in terms of the quantities $Z_j := \frac{d_j}{2\pi} + \xi_j$ and $\Delta := g^2 - Z_1Z_2$, where $\xi_j := \xi(x_j;k)$ and $g := G(x_1,x_2;k)$. The expression simplifies if the couplings are the same at the two junctions; then $\det L = 1$ and the transfer matrix is given by

$$L = \frac{1}{g}\begin{pmatrix} Z_2 + \frac{A}{C^2}\Delta & -2\frac{\Delta}{C^2} \\ C^2 - A(Z_1+Z_2) - \frac{A^2}{C^2}\Delta & \frac{A}{C^2}\Delta + Z_1 \end{pmatrix}.$$

From here one can further derive the on-shell scattering matrix [ETV01], in particular, the reflection and transmission amplitudes are

$$r = -\frac{L_{21} + ik(L_{22}-L_{11}) + k^2L_{12}}{L_{21} - ik(L_{22}+L_{11}) - k^2L_{12}}\,, \quad t = -\frac{2ik}{L_{21} - ik(L_{22}+L_{11}) - k^2L_{12}}\,;$$

they naturally depend on k through ξ and g, and satisfy $|r|^2+|t|^2 = 1$. To find these quantities for a particular Ω we may use the fact that it is compact by assumption, hence the Laplace–Beltrami operator on it has a purely discrete spectrum. We employ the eigenvalues, $\{\lambda_n\}_{n=1}^{\infty}$, numbered in ascending order and with the multiplicity taken into account, corresponding to eigenfunctions $\{\phi_n\}_{n=1}^{\infty}$ which form an orthonormal basis in $L^2(\Omega)$. The common Green function expression then gives

$$g(k) = \sum_{n=1}^{\infty} \frac{\phi_n(x_1)\overline{\phi_n(x_2)}}{\lambda_n - k^2}\,,$$

while the regularized value (10.3) can be expressed [EŠ97] as

$$\xi(x_j,k) \,=\, \sum_{n=1}^{\infty} \left(\frac{|\phi_n(x_j)|^2}{\lambda_n - k^2} - \frac{1}{4\pi n} \right) + c(\Omega)\,,$$

where the series is absolutely convergent and the constant $c(\Omega)$ depends on the manifold G. Note that a nonzero value of $c(\Omega)$ amounts in fact just to a coupling parameter renormalization: D_j has to be changed to $D_j + 2\pi c(\Omega)$.

Several examples of such a scattering has been worked out in the literature, mostly for the case when Ω is a sphere. If the coupling is chosen according to (10.2) and the leads are attached at opposite poles, the transmission probability has resonance peaks around the values λ_n where the transmission probability is close to one, and a background, dominating at high energies, which behaves as $\mathcal{O}(k^{-2}(\ln k)^{-1})$, cf. [ETV01]. Similar behavior can be demonstrated for other couplings at the junctions [Ki97]; the background suppression is faster if the junctions are not antipolar [BGMP02]. Recall also that this resonance behavior is manifested in conductance properties of such systems as a function of the electrochemical potential given by the Landauer-Büttiker formula, see, e.g., [BGMP02].

10.3. Equivalence of the resonance notions

Let us return finally to a more general situation[4] and consider a ‘hedgehog’ consisting of a two-dimensional Riemannian manifold Ω, compact, connected, and for simplicity supposed to be embedded into $\mathbb{R}^3$, endowed with a metric g_{rs}, to which a finite number n_j of half-line leads is attached at points x_j, $j = 1,\dots,n$ belonging to a finite subset $\{x_j\}$ of the interior of Ω; by $M = \sum_j n_j$ we denote the total number of the leads. The Hilbert space will be correspondingly $\mathcal{H} = L^2(\Omega, \sqrt{|g|}\,\mathrm{d}x) \oplus \bigoplus_{i=1}^{M} L^2(\mathbb{R}_+^{(i)})$.

Let H_0 be the closure of the Laplace–Beltrami operator $-g^{-1/2}\partial_r(g^{1/2}g^{rs}\partial_s)$ defined on functions from $C_0^\infty(\Omega)$; if $\partial\Omega \neq \emptyset$ we require that they satisfy there appropriate boundary conditions, either Neumann/Robin, $(\partial_n + \gamma)f|_{\partial\Omega} = 0$, or Dirichlet, $f|_{\partial\Omega} = 0$. The restriction H_0' of H_0 to the domain $\{f \in D(H_0) :\, f(x_j) =$

[4]Considerations of this section follow the paper [EL13]. Similarly one can treat ‘hedgehogs’ with three-dimensional manifolds, just replacing logarithmic singularities by polar ones.

$0,\ j = 1, \dots, n\}$ is a symmetric operator with deficiency indices (n, n). Furthermore, we denote by H_i the negative Laplacian on $L^2(\mathbb{R}_+^{(i)})$ referring to the ith lead and by H_i' its restriction to functions which vanish together with their first derivative at the half-line endpoint. The direct sum $H' = H_0' \oplus H_1' \oplus \cdots \oplus H_M'$ is obviously a symmetric operator with deficiency indices $(n+M, n+M)$.

As before admissible Hamiltonians are identified with self-adjoint extensions of the operator H' being described by the conditions (7.2) where U is now an $(n+M) \times (n+M)$ unitary matrix, I the corresponding unit matrix, and furthermore, $\Psi = (L_{1,1}(f), \dots, L_{1,n}(f), f_1(0), \dots, f_n(0))^{\mathrm{T}}$ and is Ψ' the analogous column of (generalized) boundary values with $L_{1,j}(f)$ replaced by $L_{0,j}(f)$ and $f_1(0)$ by $f_j'(0)$, respectively. The first n entries correspond to the manifold part being equal to the appropriate coefficients in the expansion of functions $f \in D(H_0^*)$ the asymptotic expansion near x_j, namely $f(x) = L_{0,j}(f) F_0(x, x_j) + L_{1,j}(f) + \mathcal{O}(r(x, x_j))$, where

$$F_0(x, x_j) = -\frac{q_2(x, x_j)}{2\pi} \ln r(x, x_j)$$

with $r(x, x_j)$ being the geodetic distance on Ω; according to Lemma 4 in [BG03] q_2 is a continuous functions of x with $q_i(x_j, x_j) = 1$. The extension described by such conditions will be denoted as H_U. We are naturally interested in *local* couplings; in analogy with considerations of Section 7.1 we can work with one 'large' matrix U and encode the junction geometry in its block structure.

Another useful thing we can adopt from the previous discussion is the possibility to employ conditions $(\tilde{U}_j(k) - I) d_j(f) + i(\tilde{U}_j(k) + I) c_j(f) = 0$ on the manifold Ω itself with the effective, energy-dependent coupling described by the matrix

$$U_j(k) = U_{1j} - (1-k) U_{2j} [(1-k) U_{4j} - (k+1) I]^{-1} U_{3j}$$

at the jth lead endpoint, where U_{1j} denotes top-left entry of U_j, U_{2j} the rest of the first row, U_{3j} the rest of the first column and U_{4j} is $n_j \times n_j$ part corresponding to the coupling between the leads attached to the manifold at the same point.

To find the on-shell scattering matrix at energy k^2 one has to couple solutions $a_j(k)\mathrm{e}^{-ikx} + b_j(k)\mathrm{e}^{ikx}$ on the leads to solution on the manifold and to look at the continuation of the result to the complex plane. On the other hand to find the resolvent singularities, we can again employ the complex scaling and to find complex eigenvalues of the resulting non-selfadjoint operator. In both cases we need the solution on the manifold; modifying the conclusions of [Ki97] mentioned above we can infer that it has to be of the form $f(x, k) = \sum_{j=1}^{n} c_j G(x, x_j; k)$,

Consider first the scattering resonances. Denoting the coefficient vector of $f(x, k)$ as $\mathbf{c}$ and using similar abbreviations $\mathbf{a}$ for the vector of the amplitudes of the incoming waves, $(a_1(k), \dots, a_M(k))^{\mathrm{T}}$, and $\mathbf{b}$ for the vector of the amplitudes of the outgoing waves, one obtains in general a system of equations,

$$A(k)\mathbf{a} + B(k)\mathbf{b} + C(k)\mathbf{c} = 0\,,$$

in which A and B are $(n+M) \times M$ matrices and C is $(n+M) \times n$ matrix the elements of which are exponentials and Green's functions, regularized if necessary;

what is important that all the entries of the mentioned matrices allow for an analytical continuation which makes it possible to ask for complex k for which the above system is solvable. For $k_0^2 \notin \mathbb{R}$ the columns of $C(k_0)$ are linearly independent and one can eliminate $\mathbf{c}$ and rewrite the above system as

$$\tilde{A}(k_0)\mathbf{a} + \tilde{B}(k_0)\mathbf{b} = 0\,,$$

where $\tilde{A}(k_0)$ and $\tilde{B}(k_0)$ are $M \times M$ matrices the entries of which are rational functions of the entries of the previous ones. If $\det \tilde{A}(k_0) = 0$ there is a solution with $\mathbf{b} = 0$, and consequently, k_0 should be an eigenvalue of H since $\operatorname{Im} k_0 < 0$ and the corresponding eigenfunction belongs to L^2, however, this contradicts to the self-adjointness of H. Next we notice that the S-matrix analytically continued to the point k_0 equals $-\tilde{B}(k_0)^{-1}\tilde{A}(k_0)$ hence its singularities must solve $\det \tilde{B}(k) = 0$.

On the other hand, for resolvent resonances we use exterior complex scaling with $\arg\theta > \arg k_0$, then the solution $a_j(k)\mathrm{e}^{-ikx}$ on the jth lead, analytically continued to the point $k = k_0$, is after the transformation by U_θ exponentially increasing, while $b_j(k)\mathrm{e}^{ikx}$ becomes square integrable. This means that solving in L^2 the eigenvalue problem for the complex-scaled operator one has to find solutions of the above system with $\mathbf{a} = 0$ which leads again to the condition $\det \tilde{B}(k) = 0$. This allows us to make the following conclusion.

Theorem 10.1. *In the described setting, the hedgehog system has a scattering resonance at k_0 with $\operatorname{Im} k_0 < 0$ and $k_0^2 \notin \mathbb{R}$ iff there is a resolvent resonance at k_0. Algebraic multiplicities of the resonances defined in both ways coincide.*

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Localization for Random Block Operators

Martin Gebert and Peter Müller

Dedicated to Michael Demuth on the occasion of his 65th birthday

Abstract. We continue the investigations of Kirsch, Metzger and the second-named author [J. Stat. Phys. **143**, 1035–1054 (2011)] on spectral properties of a certain type of random block operators. In particular, we establish an alternative version of a Wegner estimate and an improved result on Lifschitz tails at the internal band edges. Using these ingredients and the bootstrap multi-scale analysis, we also prove dynamical localization in a neighbourhood of the internal band edges.

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1. The model and its basic properties

Random block operators arise in several different fields of Theoretical Physics. In this paper we are concerned with those that are relevant to mesoscopic disordered systems such as dirty superconductors. In this context, block operators are used to describe quasi-particle excitations within the self-consistent Bogoliubov-de Gennes equations. It turns out that such block operators fall in 10 different symmetry classes [AZ97]. As in the previous paper [KMM11], we will consider one particular symmetry class, class $C1$, and refer to [KMM11] for further discussions and motivations.

Given some Hilbert space $\mathcal{H}$, we write $\mathcal{L}(\mathcal{H})$ for the Banach space of all bounded linear operators from $\mathcal{H}$ into itself. In this paper we are concerned with the Hilbert space $\mathcal{H}^2 := \ell^2(\mathbb{Z}^d) \oplus \ell^2(\mathbb{Z}^d)$, the direct sum of two Hilbert spaces of complex-valued, square-summable sequences indexed by the d-dimensional integers $\mathbb{Z}^d$. We also fix a probability space $(\Omega, \mathcal{F}, \mathbb{P})$ with corresponding expectation denoted by $\mathbb{E}$.

Definition 1.1. In this paper a *random block operator* is an operator-valued random variable

$$\mathbb{H} : \begin{array}{l} \Omega \longrightarrow \mathcal{L}(\mathcal{H}^2) \\ \omega \longmapsto \mathbb{H}^\omega := \begin{pmatrix} H^\omega & B^\omega \\ B^\omega & -H^\omega \end{pmatrix} \end{array} \tag{1.1}$$

with the following three properties:

(i) For $\mathbb{P}$-a.e. $\omega \in \Omega$ the operator $H^\omega := H_0 + V^\omega \in \mathcal{L}\big(l^2(\mathbb{Z}^d)\big)$ is the discrete random Schrödinger operator of the Anderson model. More precisely, H_0 stands for the negative discrete Laplacian on $\mathbb{Z}^d$, which is defined by

$$(H_0\psi)(n) := - \sum_{m\in\mathbb{Z}^d:\ |m-n|=1} [\psi(m) - \psi(n)] \tag{1.2}$$

for every $\psi \in \ell^2(\mathbb{Z}^d)$ and every $n \in \mathbb{Z}^d$. We always stick to the 1-norm $|n| := \sum_{j=1}^d |n_j|$ of $n = (n_1, \ldots, n_d) \in \mathbb{Z}^d$.

The random potential is induced by a given family $(\omega \mapsto V_n^\omega)_{n\in\mathbb{Z}^d}$ of i.i.d. real-valued random variables on Ω with single-site measure μ_V of compact support in $\mathbb{R}$. Thus, the multiplication operator given by

$$(V^\omega\psi)(n) := V_n^\omega \psi(n) \tag{1.3}$$

for every $\psi \in \ell^2(\mathbb{Z}^d)$ and every $n \in \mathbb{Z}^d$ is well defined and bounded for $\mathbb{P}$-a.e. $\omega \in \Omega$. Also, H^ω is self-adjoint and bounded for $\mathbb{P}$-a.e. $\omega \in \Omega$.

(ii) For $\mathbb{P}$-a.e. $\omega \in \Omega$ the operator $B^\omega \in \mathcal{L}\big(\ell^2(\mathbb{Z}^d)\big)$ is the multiplication operator induced by the family $(\omega \mapsto B_n^\omega)_{n\in\mathbb{Z}^d}$ of i.i.d. real-valued random variables on Ω with single-site measure μ_B of compact support in $\mathbb{R}$.

(iii) The family of random variables $(V_n)_{n\in\mathbb{Z}^d}$ is independent of the family $(B_n)_{n\in\mathbb{Z}^d}$.

Remarks 1.2.

(i) Conditions (i) and (ii) in Definition 1.1 imply that the random block operator $\mathbb{H}$ is $\mathbb{P}$-a.s. self-adjoint and bounded.

(ii) Block operators of the form (1.1) have a spectrum that is symmetric around 0, i.e., $E \in \mathbb{R}$ belongs to the spectrum $\sigma(\mathbb{H}^\omega)$, if and only if this is also true for $-E$ [KMM11, Lemma 2.3].

(iii) The random block operator $\mathbb{H}$ is ergodic with respect to $\mathbb{Z}^d$-translations, see [KMM11] for more details. Therefore, standard results imply the existence of a non-random closed set Σ such that $\sigma(\mathbb{H}) = \Sigma$ holds $\mathbb{P}$-a.s. [K89, K08, CL90, PF92]. This non-randomness also extends to the components in the Lebesgue decomposition of the spectrum.

In order to count eigenvalues we introduce a restriction of random block operators to bounded regions of space $\mathbb{Z}^d$. Given $L > 0$ we write $\Lambda_L :=]-L/2, L/2[^d \cap \mathbb{Z}^d$ for the discrete cube of "length L" about the origin and $\Lambda_L(n) := n + \Lambda_L$ for its shifted copy with centre $n \in \mathbb{Z}^d$.

Definition 1.3. Given a cube $\Lambda_L \subset \mathbb{Z}^d$, we define the finite-volume Hilbert space $\mathcal{H}_L^2 := \ell^2(\Lambda_L) \oplus \ell^2(\Lambda_L)$ and the *finite-volume random block operator*

$$\mathbb{H}_{\Lambda_L} \equiv \mathbb{H}_L : \begin{array}{l} \Omega \longrightarrow \mathcal{L}(\mathcal{H}_L^2) \\ \omega \longmapsto \mathbb{H}_L^\omega := \begin{pmatrix} H_L^\omega & B^\omega \\ B^\omega & -H_L^\omega \end{pmatrix} \end{array}, \tag{1.4}$$

where $H_L := H_{0,L} + V$ and $H_{0,L}$ is the discrete Laplacian on Λ_L with simple boundary conditions. Its matrix entries are given by $H_{0,L}(n,m) := \langle \delta_n, H_0 \delta_m \rangle$ for $n, m \in \Lambda_L$, with $(\delta_n)_{n\in\mathbb{Z}^d}$ denoting the canonical basis and $\langle \cdot, \cdot \rangle$ the canonical scalar product of $\ell^2(\mathbb{Z}^d)$. The random multiplication operators V and B are restricted to $\ell^2(\Lambda_L)$ in the canonical way.

Remarks 1.4.

(i) The operator $\mathbb{H}_L^\omega$ is well defined, bounded and self-adjoint for $\mathbb{P}$-a.e. $\omega \in \Omega$.

(ii) Simple boundary conditions are sufficient for most of our purposes here. We refer to [KMM11] for other useful restrictions of such types of block operators.

We write $|M|$ for the cardinality of a finite set M and introduce the normalized *finite-volume eigenvalue counting function*

$$\mathbb{N}_{\mathbb{H}_L}(E) := \frac{1}{2|\Lambda_L|} \big|\sigma(\mathbb{H}_L) \cap \,]-\infty, E]\,\big| = \frac{1}{2|\Lambda_L|} \operatorname{tr}_{\mathcal{H}_L^2} \big[1_{]-\infty,E]}(\mathbb{H}_L)\big], \tag{1.5}$$

which is a non-negative random variable for every $E \in \mathbb{R}$. Here, 1_G stands for the indicator function of a set G and $\operatorname{tr}_{\mathcal{H}}$ for the trace over some Hilbert space $\mathcal{H}$. The existence and self-averaging of the macroscopic limit of $\mathbb{N}_{\mathbb{H}_L}(E)$ is also a consequence of ergodicity.

Lemma 1.5 ([KMM11, Lemma 4.8]). *There exists a (non-random) right-continuous probability distribution function* $\mathbb{N} : \mathbb{R} \to [0,1]$*, the* integrated density of states *of* $\mathbb{H}$*, and a measurable subset* $\Omega_0 \subseteq \Omega$ *of full measure,* $\mathbb{P}(\Omega_0) = 1$*, such that*

$$\mathbb{N}(E) = \lim_{L\to\infty} \mathbb{N}_{\mathbb{H}_L}^\omega(E) = \lim_{L\to\infty} \mathbb{E}\left[\mathbb{N}_{\mathbb{H}_L}(E)\right] \tag{1.6}$$

holds for every $\omega \in \Omega_0$ *and every continuity point* $E \in \mathbb{R}$ *of* $\mathbb{N}$.

Since $\sigma(\mathbb{H}) = \Sigma$ holds $\mathbb{P}$-a.s., one can ask for the precise location of this almost-sure spectrum. A partial answer is given by

Lemma 1.6 ([KMM11, Lemma 4.3]). *Consider the random block operator* $\mathbb{H}$ *of Definition* 1.1. *Then we have* $\mathbb{P}$*-a.s.*

$$\Big\{ \pm\sqrt{E^2 + \beta^2} : E \in \sigma(H), \beta \in \operatorname{supp}(\mu_B)\Big\} \subseteq \sigma(\mathbb{H}) \subseteq [-r, r], \tag{1.7}$$

where $r := \sup_{E\in\sigma(H)} |E| + \sup_{\beta\in\operatorname{supp}(\mu_B)} |\beta|$.

We say that an interval $]a_1, a_2[$, where $a_1, a_2 \in \mathbb{R}$ with $a_1 < a_2$, is a *spectral gap* of a self-adjoint operator A, if $]a_1, a_2[\, \cap\, \sigma(A) = \varnothing$ and $a_1, a_2 \in \sigma(A)$. In order to determine the spectral gap of $\mathbb{H}$, we will combine the above lemma with a deterministic result.

Lemma 1.7 ([KMM11, Prop. 2.10]). *Consider the random block operator* $\mathbb{H}$ *of Definition* 1.1*. Then we have for* $\mathbb{P}$*-a.a.* $\omega \in \Omega$*:*

(i) *If there exists* $\lambda \geq 0$ *such that* $\inf \operatorname{supp} \mu_V \geq \lambda$*, then*

$$\sigma(\mathbb{H}^\omega) \cap \,]-\lambda, \lambda[\, = \varnothing. \tag{1.8}$$

(ii) *If there exists* $\beta \geq 0$ *such that* $\inf \operatorname{supp} \mu_B \geq \beta$*, then*

$$\sigma(\mathbb{H}^\omega) \cap \,]-\beta, \beta[\, = \varnothing. \tag{1.9}$$

(iii) *If there exist* $\lambda, \beta \geq 0$ *such that* $\inf \operatorname{supp} \mu_V \geq \lambda$ *and* $\inf \operatorname{supp} \mu_B \geq \beta$*, then*

$$\sigma(\mathbb{H}^\omega) \cap \,]-\sqrt{\lambda^2+\beta^2}, \sqrt{\lambda^2+\beta^2}[\, = \varnothing. \tag{1.10}$$

Remark 1.8. Lemmas 1.6 and 1.7 together provide the following two statements.

(i) If $\lambda := \inf \operatorname{supp} \mu_V > 0$ and $0 \in \operatorname{supp} \mu_B$, then $]-\lambda, \lambda[$ is $\mathbb{P}$-a.s. a spectral gap of $\mathbb{H}$ around 0.

(ii) If $\lambda := \inf \operatorname{supp} \mu_V \geq 0$ and $\beta := \inf \operatorname{supp} \mu_B > 0$, then $]-\sqrt{\lambda^2+\beta^2}, \sqrt{\lambda^2+\beta^2}[$ is $\mathbb{P}$-a.s. a spectral gap of $\mathbb{H}$ around 0.

For completeness and later use we review the main result of [KMM11], which is a Wegner estimate for the operator $\mathbb{H}$. In the next section we provide a new variant of this result. We write $\|f\|_{BV}$ for the total variation norm of some function $f : \mathbb{R} \to \mathbb{R}$.

Theorem 1.9 (Wegner estimate [KMM11, Thm. 5.1]). *Consider the random block operator* $\mathbb{H}$ *of Definition* 1.1 *and assume that at least one of the following conditions is met.*

(1) *There exists* $\lambda > 0$ *such that* $\inf \operatorname{supp} \mu_V \geq \lambda$ *and* μ_V *is absolutely continuous with a piecewise continuous Lebesgue density* ϕ_V *of bounded variation and compact support.*

(2) *There exists* $\beta > 0$ *such that* $\inf \operatorname{supp} \mu_B \geq \beta$ *and* μ_B *is absolutely continuous with a piecewise continuous Lebesgue density* ϕ_B *of bounded variation and compact support.*

Then the integrated density of states $\mathbb{N}$ *of* $\mathbb{H}$ *is Lipschitz continuous and has a bounded Lebesgue derivative, the density of states* $\mathbb{D} := \mathrm{d}\mathbb{N}/\mathrm{d}E$*.*

Furthermore, if hypothesis (1) *holds, then we have for Lebesgue-a.a.* $E \in \mathbb{R}$ *that*

$$\mathbb{D}(E) \leq 2\frac{|E|+1}{\lambda} \|\phi_V\|_{BV} \,. \tag{1.11}$$

In case of hypothesis (2)*, we get the estimate*

$$\mathbb{D}(E) \leq 2\frac{|E|+1}{\beta} \|\phi_B\|_{BV} \tag{1.12}$$

for Lebesgue-a.a. $E \in \mathbb{R}$*.*

2. Results

In this section we present the results of this paper. All proofs are deferred to subsequent sections. We start with a variant of Theorem 1.9.

Theorem 2.1 (Wegner estimate). *Consider the random block operator* $\mathbb{H}$ *of Definition* 1.1 *and assume that* $\inf \operatorname{supp} \mu_V \geq 0$ *and* $\inf \operatorname{supp} \mu_B \geq 0$. *Assume further that the single-site measures* μ_V *and* μ_B *are both absolutely continuous with piecewise continuous Lebesgue densities* ϕ_V, ϕ_B *of bounded variation and compact support. Then the integrated density of states* $\mathbb{N}$ *is Lipschitz continuous with a bounded Lebesgue derivative* $\mathbb{D} = \mathrm{d}\mathbb{N}/\mathrm{d}E$ *satisfying*

$$\|\mathbb{D}\|_\infty \leq 2\big(\|\phi_V\|_{BV} + \|\phi_B\|_{BV}\big). \tag{2.1}$$

Remarks 2.2.

(i) As compared to the hypotheses of the Wegner estimate from [KMM11] in Theorem 1.9, the above result constitutes an improvement in that neither H nor B have to be bounded away from 0. The price we have to pay is that *both* operators are required to be non-negative and that *both* probability distributions are assumed to be sufficiently regular.

(ii) As compared to the results of Theorem 1.9, we note that the present Wegner estimate is uniform in energy.

(iii) After completing this work, A. Elgart informed us that he can obtain a Wegner estimate for $\mathbb{H}$ which does not require assumptions on the supports of μ_V or μ_B [E12].

Next we consider the spectral asymptotics of the integrated density of states $\mathbb{N}$ of $\mathbb{H}$ at the internal band edges.

Theorem 2.3 (Internal Lifschitz tails – upper bound). *Consider the random block operator* $\mathbb{H}$ *of Definition* 1.1. *Assume that* $\lambda := \inf \operatorname{supp} \mu_V \geq 0$ *and that the support of the measure* μ_V *consists of more than a single point. Assume further that one of the following conditions is met*

(1) $\beta := \inf \operatorname{supp} \mu_B \geq 0$,

(2) $\beta := \sup \operatorname{supp} \mu_B \leq 0$,

(3) $0 \in \operatorname{supp} \mu_B$, *in which case we set* $\beta := 0$.

Then we have

$$\limsup_{\epsilon \searrow 0} \frac{\ln \Big| \ln \Big[\mathbb{N}\big(\sqrt{\lambda^2+\beta^2}+\epsilon\big) - \mathbb{N}\big(\sqrt{\lambda^2+\beta^2}\big)\Big]\Big|}{\ln \epsilon} \leq -\alpha \tag{2.2}$$

with $\alpha = d/2$ *in all cases except the case* $\lambda = 0$ *and* $\beta \neq 0$, *where* $\alpha = d/4$.

Remarks 2.4.

(i) An analogous result holds when approaching the upper edge of the lower band $-\sqrt{\lambda^2+\beta^2}$ from below.

(ii) There is no conflict in the definition of β in Theorem 2.3 if several of the conditions (1)–(3) hold, because this case is only possible with $\beta = 0$.

(iii) If $\lambda > 0$ or $\beta \neq 0$, then $\pm\sqrt{\lambda^2+\beta^2}$ are the endpoints of the spectral gap of $\mathbb{H}$; see Remark 1.8. To apply this remark in the case (2), use also unitary equivalence of $\left(\begin{smallmatrix} H & B \\ B & -H \end{smallmatrix}\right)$ and $\left(\begin{smallmatrix} H & -B \\ -B & -H \end{smallmatrix}\right)$.

(iv) Theorem 2.3 is a generalization of [KMM11, Thm. 6.1] which applies only to $\lambda > 0$ and $\beta = 0$.

A (mostly) complementary lower bound is provided by

Theorem 2.5 (Internal Lifschitz tails – lower bound). *Consider the random block operator* $\mathbb{H}$ *of Definition* 1.1. *Assume that* $\lambda := \inf \operatorname{supp} \mu_V \geq 0$ *and that one of the cases* (1)–(3) *in Theorem* 2.3 *applies. Assume further the existence of constants* $C, \kappa > 0$ *such that for all sufficiently small* $\eta > 0$ *the bounds*

$$\mu_V\big([\lambda, \lambda+\eta[\big) \geq C\eta^{\kappa} \qquad \textit{and} \qquad \mu_B\big(]\beta-\eta, \beta+\eta[\big) \geq C\eta^{\kappa} \tag{2.3}$$

hold. Then we have

$$\liminf_{\epsilon \searrow 0} \frac{\ln\Big|\ln\Big[\mathbb{N}\big(\sqrt{\lambda^2+\beta^2}+\epsilon\big) - \mathbb{N}\big(\sqrt{\lambda^2+\beta^2}\big)\Big]\Big|}{\ln \epsilon} \geq -d/2. \tag{2.4}$$

Remarks 2.6.

(i) Taken together, Theorems 2.3 and 2.5 imply that the random block operator $\mathbb{H}$ exhibits Lifschitz tails at the edges of its spectral gap with Lifschitz exponent $d/2$ for all values $\lambda > 0$ and $\beta \in \mathbb{R}$.

(ii) Even in the case $\lambda = \beta = 0$, the block operator $\mathbb{H}$ exhibits Lifschitz tails with Lifschitz exponent $d/2$ at energy zero. We note that there is no internal spectral edge at energy zero in this case.

(iii) In the case $\lambda = 0$ and $\beta \neq 0$ we believe that the correct value of the Lifschitz exponent is $d/2$ (rather than $d/4$), as given by the lower bound in Theorem 2.5.

Finally, we turn to the Anderson localization of $\mathbb{H}$ in a neighbourhood of the internal band edges. The following notion will be useful for the formulation of the result.

Definition 2.7. Given a bounded operator $\mathbb{A}$ on the Hilbert space $\mathcal{H}^2$ and $n, m \in \mathbb{Z}^d$, we introduce its 2×2-matrix-valued matrix element

$$\mathbb{A}(n,m) := \begin{pmatrix} \left\langle\!\!\left\langle \begin{pmatrix}\delta_n\\0\end{pmatrix}, \mathbb{A}\begin{pmatrix}\delta_m\\0\end{pmatrix}\right\rangle\!\!\right\rangle & \left\langle\!\!\left\langle \begin{pmatrix}\delta_n\\0\end{pmatrix}, \mathbb{A}\begin{pmatrix}0\\\delta_m\end{pmatrix}\right\rangle\!\!\right\rangle \\ \left\langle\!\!\left\langle \begin{pmatrix}0\\\delta_n\end{pmatrix}, \mathbb{A}\begin{pmatrix}\delta_m\\0\end{pmatrix}\right\rangle\!\!\right\rangle & \left\langle\!\!\left\langle \begin{pmatrix}0\\\delta_n\end{pmatrix}, \mathbb{A}\begin{pmatrix}0\\\delta_m\end{pmatrix}\right\rangle\!\!\right\rangle \end{pmatrix}. \tag{2.5}$$

Here $\langle\!\langle \cdot, \cdot \rangle\!\rangle$ stands for the canonical scalar product on the Hilbert space $\mathcal{H}^2$. We also fix some norm $\|\cdot\|_{2\times 2}$ on the vector space of complex-valued 2×2-matrices.

Theorem 2.8 (Complete localization). *Consider the random block operator* $\mathbb{H}$ *of Definition* 1.1 *and assume the hypotheses of Theorem* 2.3. *Assume further the hypotheses of Theorem* 1.9 *or Theorem* 2.1. *Then there exist constants* $0 < \zeta < 1$, $C_\zeta > 0$ *and an energy interval* $I := [-a, a]$, *where* $a > 0$, *such that* $I \cap \sigma(\mathbb{H}) \neq \varnothing$ *holds* $\mathbb{P}$*-a.s. and*

$$\mathbb{E}\left(\sup_{\|f\|_\infty \le 1} \left\| \big(1_I(\mathbb{H}) f(\mathbb{H})\big)(n,m) \right\|_{2\times 2}\right) \le C_\zeta \, \mathrm{e}^{-|n-m|^\zeta} \tag{2.6}$$

for all $n, m \in \mathbb{Z}^d$. *The supremum in* (2.6) *is taken over all Borel functions* $\mathbb{R} \to \mathbb{C}$ *that are pointwise bounded by* 1.

Remark 2.9.

(i) The choice of the matrix norm $\|\cdot\|_{2\times 2}$ is not crucial here. It can be replaced by any other matrix norm on the space of 2×2 matrices.

(ii) Our proof of the theorem relies on the bootstrap multi-scale analysis of Germinet and Klein [GK01]. In fact, the general formulation of the bootstrap multi-scale analysis in [GK01] allows an immediate and straightforward application to the present setting of random block operators. An alternative proof of localization has been carried out previously in [ESS12]. It adapts the fractional-moment method to rather general $k \times k$-block operators for $k \geq 2$ and applies in the strong-disorder regime. We would like to advertise the simplicity of extending the bootstrap multi-scale analysis to our block-operator setting.

(iii) Further equivalent characterizations of the region of complete localization can be found in [GK04, GK06].

The RAGE Theorem leads to the following well-known corollary of Theorem 2.8.

Corollary 2.10 (Spectral localization). *Under the assumptions of Theorem* 2.8 *there is only pure point spectrum in* I, *that is*

$$\sigma(\mathbb{H}) \cap I = \sigma_{\mathrm{pp}}(\mathbb{H}) \cap I \tag{2.7}$$

holds $\mathbb{P}$*-a.s., and the eigenfunctions of* $\mathbb{H}$ *associated with eigenvalues in* I *decay exponentially at infinity.*

3. Proof of the Wegner estimate

The following proof of Theorem 2.1 is close to the one given in [KMM11], the main difference being Lemma 3.1 below.

Proof of Theorem 2.1. In order to stress the dependence of the finite-volume operator on the families of random variables $V := (V_n)_{n\in\mathbb{Z}^d}$ and $B := (B_n)_{n\in\mathbb{Z}^d}$, we use the notation $\mathbb{H}_L \equiv \mathbb{H}_L(V,B)$ whenever appropriate. Since

$$\mathbb{P}\left(\text{all eigenvalues of } \mathbb{H}_L \text{ are non-degenerate}\right) = 1, \tag{3.1}$$

see, e.g., [KS80, Prop. II.1], we infer from analytic perturbation theory that for $\mathbb{P}$-a.e. (V,B) the distinct eigenvalues $E_j \equiv E_j(V,B)$, $j = 1,\ldots,2|\Lambda_L|$, of $\mathbb{H}_L(V,B)$, which are ordered by magnitude, are all continuously differentiable (separately in each V_n and each B_n for $n = 1,\ldots,|\Lambda_L|$) in the point (V,B). For the time being we fix $E > 0$ and $\epsilon > 0$ with $3\epsilon < E$. Consider a switch function $\rho \in C^1(\mathbb{R})$, i.e., ρ is continuously differentiable, non-decreasing and obeys $0 \le \rho \le 1$, with $\rho(\eta) = 1$ for $\eta > \epsilon$ and $\rho(\eta) = 0$ for $\eta < -\epsilon$. Monotonicity gives the estimate

$$\begin{aligned}\operatorname{tr}_{\mathcal{H}_L^2}\left[1_{[E-\epsilon,E+\epsilon[}(\mathbb{H}_L)\right] &\le \sum_{j=1}^{2|\Lambda_L|}\left[\rho\left(E_j - E + 2\epsilon\right) - \rho\left(E_j - E - 2\epsilon\right)\right] \\ &= \int_{E-2\epsilon}^{E+2\epsilon} \mathrm{d}\eta \sum_{j=1}^{2|\Lambda_L|} \rho'\left(E_j - \eta\right).\end{aligned} \tag{3.2}$$

We infer from the chain rule that

$$\begin{aligned}&\sum_{n\in\Lambda_L}\left(\frac{\partial}{\partial V_n} + \frac{\partial}{\partial B_n}\right)\rho\big(E_j(V,B) - \eta\big) \\ &\quad = \rho'\big(E_j(V,B) - \eta\big)\sum_{n\in\Lambda_L}\left(\frac{\partial}{\partial V_n} + \frac{\partial}{\partial B_n}\right)E_j(V,B)\end{aligned} \tag{3.3}$$

for all j, all η and $\mathbb{P}$-a.a. (V,B). Unlike the standard Anderson model, the eigenvalues $E_j(V,B)$ are neither monotone in the V_n's nor in the B_n's, but the choice of ϵ ensures that only positive eigenvalues contribute to the j-sum in (3.2). Therefore we apply Lemma 3.1 to (3.3), and estimate ρ' in (3.2) according to

$$\rho'\big(E_j(V,B) - \eta\big) \le \sum_{n\in\Lambda_L}\left(\frac{\partial}{\partial V_n} + \frac{\partial}{\partial B_n}\right)\rho\big(E_j(V,B) - \eta\big). \tag{3.4}$$

Taking the expectation of (3.2) and using its product structure, we obtain

$$\begin{aligned}&\mathbb{E}\Big\{\operatorname{tr}_{\mathcal{H}_L^2}\left[1_{[E-\epsilon,E+\epsilon[}(\mathbb{H}_L)\right]\Big\} \\ &\quad\le \int_{E-2\epsilon}^{E+2\epsilon}\mathrm{d}\eta \sum_{n\in\Lambda_L}\int_{\mathbb{R}^{2|\Lambda_L|}}\Big(\prod_{k\in\Lambda_L}\mathrm{d}\mu_V(V_k)\,\mathrm{d}\mu_B(B_k)\Big) \\ &\qquad\times\sum_{j=1}^{2|\Lambda_L|}\left(\frac{\partial}{\partial V_n} + \frac{\partial}{\partial B_n}\right)\rho\big(E_j(V,B) - \eta\big).\end{aligned} \tag{3.5}$$

Each term of the n-sum in the previous expression can be rewritten as

$$\begin{aligned}\int_{\mathbb{R}^{2|\Lambda_L|-2}}&\bigg(\prod_{k\in\Lambda_L:\ k\neq n}\mathrm{d}\mu_V(V_k)\,\mathrm{d}\mu_B(B_k)\bigg)\\ &\times\bigg[\int_{\mathbb{R}}\mathrm{d}\mu_B(B_n)\int_{\mathbb{R}}\mathrm{d}\mu_V(V_n)\sum_{j=1}^{2|\Lambda_L|}\frac{\partial}{\partial V_n}\rho\big(E_j(V,B)-\eta\big)\\ &\qquad+\int_{\mathbb{R}}\mathrm{d}\mu_V(V_n)\int_{\mathbb{R}}\mathrm{d}\mu_B(B_n)\sum_{j=1}^{2|\Lambda_L|}\frac{\partial}{\partial B_n}\rho\big(E_j(V,B)-\eta\big)\bigg].\end{aligned}\tag{3.6}$$

Functions like $X_n\mapsto F(X_n):=\sum_{j=1}^{2|\Lambda_L|}\rho\big(E_j(V,B)-\eta\big)$, where X stands for V or B, are non-monotone in general. But analytic perturbation theory ensures that $F\in C^1(\mathbb{R})$. Moreover, $|F(x)-F(x')|\leq 2$ for all $x,x'\in\mathbb{R}$ by a rank-2-perturbation argument. Therefore, Lemma 5.4. in [KMM11] implies

$$\int_{\mathbb{R}}\mathrm{d}\mu_X(X_n)\sum_{j=1}^{2|\Lambda_L|}\frac{\partial}{\partial X_n}\rho\big(E_j(V,B)-\eta\big)\leq 2\,\|\phi_X\|_{BV}\tag{3.7}$$

for both $X=V$ and $X=B$. Thus, we conclude from (3.5)–(3.7) that

$$\mathbb{E}\Big\{\operatorname{tr}_{\mathcal{H}_L^2}\big[1_{[E-\epsilon,E+\epsilon[}(\mathbb{H}_L)\big]\Big\}\leq 8\epsilon\,|\Lambda_L|\,\big(\|\phi_V\|_{BV}+\|\phi_B\|_{BV}\big)\tag{3.8}$$

for every $E>0$ and every $0<\epsilon<E/3$. This bound and dominated convergence establish Lipschitz continuity of the integrated density of states $\mathbb{N}$ on $\mathbb{R}_{>0}$ with Lipschitz constant $2\,(\|\phi_V\|_{BV}+\|\phi_B\|_{BV})$. But due to the symmetry of the spectrum, see Remark 1.2(ii), this extends to $\mathbb{R}\setminus\{0\}$. Furthermore, since $\mathbb{N}$ is a continuous function on the whole real line $\mathbb{R}$ – which follows from standard arguments as in [K08, Thm. 5.14] – this yields Lipschitz continuity on $\mathbb{R}$ with the same constant. □

One of the main estimates in the previous proof is provided by the following deterministic result.

Lemma 3.1. *Assume that $H_L\geq 0$, $B_L\geq 0$ and let $E(V,B)>0$ be a simple eigenvalue of $\mathbb{H}_L(V,B)$. Then we have*

$$\sum_{n\in\Lambda_L}\left(\frac{\partial}{\partial V_n}+\frac{\partial}{\partial B_n}\right)E(V,B)\geq 1.\tag{3.9}$$

Proof. Let $\Psi=(\psi_1,\psi_2)$ be a normalized eigenvector corresponding to the eigenvalue $E\equiv E(V,B)$ of the operator $\mathbb{H}_L\equiv\mathbb{H}_L(V,B)$, i.e., $\langle\psi_1,\psi_1\rangle+\langle\psi_2,\psi_2\rangle=1$ and

$$\begin{aligned}H_L\psi_1+B\psi_2&=E\psi_1,\\ B\psi_1-H_L\psi_2&=E\psi_2.\end{aligned}\tag{3.10}$$

The Feynman-Hellmann formula for a non-degenerate eigenvalue and (3.10) imply

$$\begin{aligned} E &\sum_{j\in\Lambda_L} \left(\frac{\partial}{\partial V_j} + \frac{\partial}{\partial B_j}\right) E \\ &= E\left(\langle\psi_1,\psi_1\rangle - \langle\psi_2,\psi_2\rangle + \langle\psi_1,\psi_2\rangle + \langle\psi_2,\psi_1\rangle\right) \\ &= \langle\psi_1, H_L\psi_1 + B\psi_2\rangle - \langle B\psi_1 - H_L\psi_2, \psi_2\rangle + \langle\psi_1, B\psi_1 - H_L\psi_2\rangle \\ &\quad + \langle\psi_2, H_L\psi_1 + B\psi_2\rangle \\ &= \langle\psi_1, H_L\psi_1\rangle + \langle\psi_2, H_L\psi_2\rangle + \langle\psi_1, B\psi_1\rangle + \langle\psi_2, B\psi_2\rangle\,. \end{aligned} \tag{3.11}$$

In the last step we used that the operator $\mathbb{H}_L$ is a real symmetric matrix and, therefore, the eigenvector Ψ can be chosen to be real. Since $B \geq 0$, we have

$$\langle\psi_1, B\psi_1\rangle + \langle\psi_2, B\psi_2\rangle \geq \langle\psi_1, B\psi_2\rangle + \langle\psi_2, B\psi_1\rangle\,. \tag{3.12}$$

This and $H_L \geq 0$ yield the lower bound

$$\langle\psi_1, H_L\psi_1 + B\psi_2\rangle + \langle\psi_2, B\psi_1 - H_L\psi_2\rangle = E\left(\langle\psi_1,\psi_1\rangle + \langle\psi_2,\psi_2\rangle\right) = E \tag{3.13}$$

for the r.h.s. of (3.11). □

4. Proof of Lifschitz tails

In this section we prove Theorems 2.3 and 2.5.

The idea behind the proof of Theorem 2.3 is to estimate the integrated density of states of $\mathbb{H}$ in terms of the integrated density of states of the operator

$$\mathbb{H}(\beta) := \begin{pmatrix} H & \beta\mathbf{1} \\ \beta\mathbf{1} & -H \end{pmatrix}, \tag{4.1}$$

on $\mathcal{H}^2$, where β is as in Theorem 2.3 and $\mathbf{1}$ denotes the unit operator on $\ell^2(\mathbb{Z}^d)$. This is useful because we explicitly know the relation between the spectra of $\mathbb{H}(\beta)$ and H, and because the discrete Schrödinger operator H of the Anderson model exhibits Lifschitz tails at the edges of its spectrum. For the lower spectral edge of H the upper Lifschitz-tail estimate is summarized in the next lemma, for a proof see, e.g., [CL90, PF92, K89].

Lemma 4.1 (Upper Lifschitz-tail estimate for H). *Let H be the discrete random Schrödinger operator of the Anderson model as in Definition* 1.1*. Assume in addition that the single-site probability measure μ_V is not concentrated in a single point. Then, the integrated density of states N_H of the operator H obeys*

$$\limsup_{\epsilon\searrow 0} \frac{\ln|\ln[N_H(\lambda+\epsilon)]|}{\ln\epsilon} \leq -\frac{d}{2}, \tag{4.2}$$

where $\lambda := \inf\operatorname{supp}\mu_V = \inf\sigma(H)$ is the infimum of the almost-sure spectrum of H.

The remaining arguments needed for the proof of Theorem 2.3 are all deterministic. The next lemma, which is a particular case of [T08, Thm. 1.9.1], provides a variational principle for the positive spectrum of the finite-volume block operator $\mathbb{H}_L$.

Lemma 4.2 (Min-max-max principle). *Given A, B and D self adjoint operators on $\mathcal{H} = l^2(\Lambda_L)$ with $A > -D$, define the block operator $\mathbb{A} := \begin{pmatrix} A & B \\ B & -D \end{pmatrix}$ on $\mathcal{H}^2$. Then*

(i) *there are precisely $|\Lambda_L|$ eigenvalues of $\mathbb{A}$, $\lambda_1, \dots, \lambda_{|\Lambda_L|}$, with $\lambda_j > \sup \sigma(-D)$ and*
(ii) *the eigenvalues $\lambda_j > \sup \sigma(-D)$, $j = 1, \dots, |\Lambda_L|$, ordered by magnitude and repeated according to their multiplicity, are given by*

$$\lambda_j = \min_{\substack{\mathcal{V} \subset \ell^2(\Lambda_L): \\ \dim \mathcal{V} = j}} \max_{\substack{f \in \mathcal{V}: \\ \|f\|=1}} \max_{\substack{g \in \ell^2(\Lambda_L): \\ \|g\|=1}} \left\{ \frac{\langle f, Af\rangle - \langle g, Dg\rangle}{2} + \sqrt{\left(\frac{\langle f, Af\rangle + \langle g, Dg\rangle}{2} \right)^2 + |\langle f, Bg\rangle|^2} \right\}. \tag{4.3}$$

This variational characterization will serve to relate the positive spectrum of $\mathbb{H}_L$ to that of $\mathbb{H}_L(\beta)$, which is the restriction of $\mathbb{H}(\beta)$ to $\mathcal{H}_L^2$ in analogy with Definition 1.3. Finally, we relate the spectrum of $\mathbb{H}_L(\beta)$ to that of its diagonal block H_L.

Lemma 4.3 ([KMM11, Prop. 3.1]). *The spectrum of $\mathbb{H}_L(\beta)$ is given by*

$$\sigma\big(\mathbb{H}_L(\beta)\big) = \big\{ \pm \sqrt{E^2 + \beta^2} : \ E \in \sigma(H_L) \big\}. \tag{4.4}$$

Now we are prepared for the

Proof of Theorem 2.3. Since $H \geq 0$ we have $H_L > 0$ and can apply Lemma 4.2. Setting $f = g$ there and noting that $\mathbb{P}$-a.s. $\beta = \inf \sigma(|B|)$, we infer

$$\begin{aligned} \lambda_j &\geq \min_{\substack{\mathcal{V} \subset \ell^2(\Lambda_L): \\ \dim \mathcal{V} = j}} \max_{\substack{f \in \mathcal{V}: \\ \|f\|=1}} \sqrt{\langle f, H_L f\rangle^2 + \langle f, Bf\rangle^2} \\ &\geq \min_{\substack{\mathcal{V} \subset \ell^2(\Lambda_L): \\ \dim \mathcal{V} = j}} \max_{\substack{f \in \mathcal{V}: \\ \|f\|=1}} \sqrt{\langle f, H_L f\rangle^2 + \beta^2} \\ &= \left[\left(\min_{\substack{\mathcal{V} \subset \ell^2(\Lambda_L): \\ \dim \mathcal{V} = j}} \max_{\substack{f \in \mathcal{V}: \\ \|f\|=1}} \langle f, H_L f\rangle \right)^2 + \beta^2 \right]^{1/2} \end{aligned} \tag{4.5}$$

for every $j = 1, \dots, |\Lambda_L|$. We denote the positive eigenvalues of $\mathbb{H}_L(\beta)$ by $0 < \mu_1 \leq \dots \leq \mu_{|\Lambda_L|}$. The min-max principle for H_L and Lemma 4.3 then imply

$$\lambda_j \geq \mu_j \tag{4.6}$$

for every $j = 1, \ldots, |\Lambda_L|$. Symmetry of the spectra of $\mathbb{H}_L$ and $\mathbb{H}_L(\beta)$, see Remark 1.2(ii), the strict positivity $H_L > \inf \sigma(H) = \lambda \geq 0$ and Lemma 1.7(iii) imply

$$\mathbb{N}_{\mathbb{H}_L}\big(\sqrt{\lambda^2+\beta^2}\big) = \mathbb{N}_{\mathbb{H}_L(\beta)}\big(\sqrt{\lambda^2+\beta^2}\big) = \frac{1}{2}. \tag{4.7}$$

Setting $E := \sqrt{\lambda^2+\beta^2} + \epsilon$ for $\epsilon > 0$, Equations (4.7) and (4.6) give the estimate

$$\begin{aligned}
&\mathbb{N}_{\mathbb{H}_L}(E) - \mathbb{N}_{\mathbb{H}_L}\big(\sqrt{\lambda^2+\beta^2}\big) \\
&\quad \leq \mathbb{N}_{\mathbb{H}_L(\beta)}(E) - \mathbb{N}_{\mathbb{H}_L(\beta)}\big(\sqrt{\lambda^2+\beta^2}\big) \\
&\quad = \frac{1}{2|\Lambda_L|}\,\big|\big\{\,\mu \in \sigma\big(\mathbb{H}_L(\beta)\big) :\ \mu \in \big[\sqrt{\lambda^2+\beta^2}, E\big[\ \big\}\big| \\
&\quad = \frac{1}{2|\Lambda_L|}\,\big|\big\{\widetilde{\mu} \in \sigma(H_L) :\ \widetilde{\mu} \in \big[\lambda, \sqrt{E^2-\beta^2}\big[\ \big\}\big| \\
&\quad = \frac{1}{2}\,N_{H_L}\big(\sqrt{E^2-\beta^2}\big),
\end{aligned} \tag{4.8}$$

where we have used Lemma 4.3 for the second equality. Therefore we get in the limit $L \to \infty$ and using Lemma 4.1

$$\begin{aligned}
&\limsup_{\epsilon \searrow 0} \frac{\ln\big|\ln\big[\mathbb{N}(\sqrt{\lambda^2+\beta^2}+\epsilon) - \mathbb{N}(\sqrt{\lambda^2+\beta^2})\big]\big|}{\ln \epsilon} \\
&\quad \leq \limsup_{\epsilon \searrow 0} \frac{\ln\Big|\ln N_H\Big(\big[(\sqrt{\lambda^2+\beta^2}+\epsilon)^2 - \beta^2\big]^{1/2}\Big)\Big|}{\ln \epsilon} \\
&\quad = \limsup_{\widetilde{\epsilon} \searrow 0} \frac{\ln|\ln N_H(\lambda + \widetilde{\epsilon})|}{\xi \ln \widetilde{\epsilon}} \\
&\quad \leq -\frac{d}{2\,\xi}
\end{aligned} \tag{4.9}$$

with $\xi = 1$ in all cases except the case of $\lambda = 0$ and $\beta \neq 0$, where $\xi = 2$. □

In the remaining part of this section we turn to the lower bound for Lifschitz tails.

Proof of Theorem 2.5. We use the Dirichlet-Neumann bracketing. Therefore we define, following [KMM11, Def. 4.6], the *Dirichlet-bracketing* restriction of the block operator as

$$\mathbb{H}_L^{+} := \begin{pmatrix} H_L^D & B \\ B & -H_L^N \end{pmatrix}, \tag{4.10}$$

where H_L^N and H_L^D denote the restriction of H to the cube Λ_L, $L \in \mathbb{N}$, with Neumann, respectively Dirichlet boundary conditions on the Laplacian; for a precise definition see [K08, Sect. 5.2]. Setting $\widetilde{H}_L^D := H_L^D - \lambda \mathbf{1}$, $\widetilde{B} := B - \beta \mathbf{1}$ and using

Lemma 4.2, we obtain for the jth positive eigenvalue, $j = 1, \dots, |\Lambda_L|$,

$$\lambda_j(\mathbb{H}_L^D) = \min_{\substack{\mathcal{V} \subset \ell^2(\Lambda_L): \\ \dim \mathcal{V} = j}} \max_{\substack{f \in \mathcal{V}: \\ \|f\|=1}} \max_{g \in \ell^2(\Lambda_L): \|g\|=1} \Bigg\{ \frac{\langle f, \widetilde{H}_L^D f\rangle - \langle g, \widetilde{H}_L^N g\rangle}{2} + \sqrt{\bigg(\lambda + \frac{\langle f, \widetilde{H}_L^D f\rangle + \langle g, \widetilde{H}_L^N g\rangle}{2}\bigg)^2 + \big|\beta + \langle f, \widetilde{B} g\rangle\big|^2} \Bigg\}. \tag{4.11}$$

The elementary inequality

$$\sqrt{(\lambda + a)^2 + (\beta + b)^2} \leq \sqrt{\lambda^2 + \beta^2} + a + b \tag{4.12}$$

holds for every $a, b \geq 0$ and $\lambda, \beta \in \mathbb{R}$.
Together with the estimate $\big|\beta + \langle f, \widetilde{B} g\rangle\big| \leq |\beta| + \langle f, \widetilde{B}^2 f\rangle^{1/2}$, this yields

$$\lambda_j(\mathbb{H}_L^D) \leq \sqrt{\lambda^2 + \beta^2} + \min_{\substack{\mathcal{V} \subset \ell^2(\Lambda_L): \\ \dim \mathcal{V} = j}} \max_{\substack{f \in \mathcal{V}: \\ \|f\|=1}} \Big\{ \langle f, \widetilde{H}_L^D f\rangle + \langle f, \widetilde{B}^2 f\rangle^{1/2} \Big\}. \tag{4.13}$$

On the other hand, (4.11) implies

$$\lambda_j(\mathbb{H}_L^D) > \sqrt{\lambda^2 + \beta^2} \tag{4.14}$$

for every $j = 1, \dots, |\Lambda_L|$.

From this and Lemma 4.2 we conclude that $\mathbb{E}\big[\mathbb{N}_{\mathbb{H}_L^+}(\sqrt{\lambda^2 + \beta^2})\big] = 1/2$. Similarly, using the symmetry of the spectrum and continuity of the integrated density of states (cf. the proof of [K08, Lemma 5.13]), we obtain $\mathbb{E}\big[\mathbb{N}(\sqrt{\lambda^2 + \beta^2})\big] = 1/2$. These two equalities and the estimate $\mathbb{N}(E) \geq \mathbb{E}\big[\mathbb{N}_{\mathbb{H}_L^+}(E)\big]$ for every $E \in \mathbb{R}$ [KMM11, Lemma 4.8(ii)] yield

$$\begin{aligned} &\mathbb{N}(\sqrt{\lambda^2 + \beta^2} + \epsilon) - \mathbb{N}(\sqrt{\lambda^2 + \beta^2}) \\ &\quad \geq \mathbb{E}\big[\mathbb{N}_{\mathbb{H}_L^+}(\sqrt{\lambda^2 + \beta^2} + \epsilon)\big] - \mathbb{E}\big[\mathbb{N}_{\mathbb{H}_L^+}(\sqrt{\lambda^2 + \beta^2})\big] \\ &\quad \geq \frac{1}{2|\Lambda_L|} \, \mathbb{P}\Big(\lambda_1(\mathbb{H}_L^D) \in [\sqrt{\lambda^2 + \beta^2}, \sqrt{\lambda^2 + \beta^2} + \epsilon[\Big) \\ &\quad \geq \frac{1}{2|\Lambda_L|} \, \mathbb{P}\Big(\langle \psi, \widetilde{H}_L^D \psi\rangle + \langle \psi, \widetilde{B}^2 \psi\rangle^{1/2} < \epsilon\Big) \end{aligned} \tag{4.15}$$

for every $L \in \mathbb{N}$, $\epsilon > 0$ and every normalized test function $\psi \in l^2(\Lambda_L)$.

Following [K08, Sect. 6.3], we choose $\psi := \frac{1}{\|\psi_1\|}\psi_1(n)$, where $\psi_1(n) := \frac{L}{2} - |n|_\infty$ for $n \in \Lambda_L$. This implies $\langle \psi, H_{0,L}^D \psi\rangle \leq c_0 L^{-2}$ with some constant $c_0 > 0$. Next we choose L to be the smallest integer such that

$$c_0 L^{-2} < \epsilon/2 \tag{4.16}$$

and estimate

$$
\begin{aligned}
&\mathbb{P}\Big(\langle\psi, \widetilde{H}_L^D\psi\rangle + \langle\psi, \widetilde{B}^2\psi\rangle^{1/2} < \epsilon\Big)\\
&\quad\geq \mathbb{P}\left(\langle\psi, (V-\lambda\mathbf{1})\psi\rangle + \langle\psi, (B-\beta\mathbf{1})^2\psi\rangle^{1/2} < \epsilon/2\right)\\
&\quad\geq \mathbb{P}\Big(\forall\, n \in \Lambda_L:\ V(n) - \lambda < \epsilon/4 \ \text{ and }\ |B(n)-\beta| < \epsilon/4\Big)\\
&\quad= \big\{\mu_V\big([\lambda, \lambda+\epsilon/4[\big)\big\}^{|\Lambda_L|}\,\big\{\mu_B\big([\beta-\epsilon/4, \beta+\epsilon/4[\big)\big\}^{|\Lambda_L|}.
\end{aligned}
\tag{4.17}
$$

The theorem now follows with (4.15) and the assumption (2.3). □

5. Proof of localization

Our proof relies on the bootstrap multi-scale analysis introduced in [GK01], which yields complete localization in a rather general setting. Apart from one natural adaptation for multiplication operators – see below – we are only left to check whether the assumptions on the random operator are fulfilled by our model. We start with some notions.

Definition 5.1. We introduce the *boundary* of a cube $\Lambda \subset \mathbb{Z}^d$ by

$$\partial\Lambda := \big\{(n,m) \in \mathbb{Z}^d \times \mathbb{Z}^d:\ |n-m| = 1,\ n \in \Lambda,\ m \notin \Lambda \ \text{ or }\ n \notin \Lambda,\ m \in \Lambda\big\}, \tag{5.1}$$

its *inner boundary* by

$$\partial^i\Lambda := \big\{n \in \Lambda : \exists\, m \notin \Lambda \text{ such that } |n-m| = 1\big\} \tag{5.2}$$

and its *outer boundary* by

$$\partial^o\Lambda := \big\{n \notin \Lambda : \exists\, m \in \Lambda \text{ such that } |n-m| = 1\big\}. \tag{5.3}$$

We write $\Lambda_1 \sqsubset \Lambda_2$ if $\partial\Lambda_1 \subset \Lambda_2 \times \Lambda_2$. Furthermore for $\Lambda_1 \sqsubset \Lambda_2 \subseteq \mathbb{Z}^d$ we define the *boundary operator* $\Gamma_{\Lambda_1}^{\Lambda_2} \equiv \Gamma_{\Lambda_1}$ on $\ell^2(\Lambda_2)$ in terms of its matrix elements

$$\langle\delta_n, \Gamma_{\Lambda_1}\delta_m\rangle := \begin{cases} -1, & (n,m) \in \partial\Lambda_1,\\ 0, & (n,m) \in (\Lambda_2 \times \Lambda_2) \setminus \partial\Lambda_1. \end{cases} \tag{5.4}$$

We lift Γ_{Λ_1} to a bounded operator on $\ell^2(\Lambda_2) \oplus \ell^2(\Lambda_2)$ by setting

$$\mathbb{\Gamma}_{\Lambda_1} := \Gamma_{\Lambda_1} \oplus (-\Gamma_{\Lambda_1}). \tag{5.5}$$

In contrast, given subsets $\Lambda \subset \Lambda' \subseteq \mathbb{Z}^d$, we lift the multiplication operator 1_Λ on $\ell^2(\Lambda')$, corresponding to the indicator function of Λ, to the sum space $\ell^2(\Lambda') \oplus \ell^2(\Lambda')$ by setting

$$\mathbb{1}_\Lambda := 1_\Lambda \oplus 1_\Lambda. \tag{5.6}$$

In slight abuse of notation we also write $\mathbb{1}_n := \mathbb{1}_{\{n\}}$ for $n \in \mathbb{Z}^d$. Finally, given an energy $E \notin \sigma(\mathbb{H}_\Lambda)$, we use the abbreviation $\mathbb{G}_\Lambda(E) := (\mathbb{H}_\Lambda - E)^{-1}$ for the resolvent of $\mathbb{H}_\Lambda$.

Proof of Theorem 2.8. We apply [GK01, Thm. 3.8] on the Hilbert space $\mathcal{H}^2$, with the random operator $\mathbb{H}$ and with $\mathbb{1}_\Lambda$ playing the role of the multiplication operator χ_Λ in [GK01]. The deterministic Assumptions *SLI* and *EDI* will be checked in Lemmas 5.2 and 5.3 below. We note a slight structural difference between the statement of Lemma 5.3 and the *EDI*-property in [GK01]: the factor $\|\mathbb{1}_{\partial^o\Lambda}\Psi\|$ in (5.12) evaluates Ψ outside the cube Λ. However, this factor plays only a role in the proof of Lemma 4.1 in [GK01], and Eq. (4.3)–(4.4) in that proof show that this difference is irrelevant.

The next important hypothesis of Theorem 3.8 in [GK01] is the Wegner Assumption *W*, which follows from Theorem 1.9 or 2.1 for our model with $b = 1$ (more precisely from the finite-volume estimates – e.g., (3.8) – in the proofs of those theorems). The remaining assumptions *IAD*, *NE* and *SGEE* are obviously correct because we work with a discrete model with i.i.d. random coupling constants. Finally, the initial-scale estimate follows from Theorem 5.5 below, see also Remark 3.7 in [GK01].

Having collected all the aforementioned properties, Corollary 3.12 of [GK01] implies that the claim of Theorem 3.8 in [GK01] holds for all energies in some interval $I := [-a, a]$, where $a > \sqrt{\lambda^2 + \beta^2}$ so that I overlaps with the almost-sure spectrum of $\mathbb{H}$ according to Lemma 1.6. The claim of Theorem 3.8 in [GK01] then reads

$$\mathbb{E}\left(\sup_{\|f\|_\infty \le 1} \left\|\mathbb{1}_n 1_I(\mathbb{H}) f(\mathbb{H}) \mathbb{1}_m\right\|_{HS}^2\right) \le C_\zeta\, \mathrm{e}^{-|n-m|^\zeta} \tag{5.7}$$

for all $n, m \in \mathbb{Z}^d$. Here, $\|\mathbb{A}\|_{HS}$ is the Hilbert–Schmidt norm of an operator $\mathbb{A}$ on $\mathcal{H}^2$. To get to our formulation in (2.6) we remark that

$$\|\mathbb{1}_n \mathbb{A} \mathbb{1}_m\|_{HS} = \|\mathbb{A}(n,m)\|_{2\times 2}, \tag{5.8}$$

where, on the right-hand side, we use the notation introduced in (2.5), and $\|\cdot\|_{2\times 2}$ stands for the Hilbert–Schmidt norm of a 2×2-matrix. Replacing the latter by any other norm on the 2×2-matrices as in (2.6), merely requires a possible adjustment of the constant C_ζ. □

Next we deal with the deterministic assumptions required by the bootstrap multi-scale analysis. The first one is a consequence of the geometric resolvent equation (5.11).

Lemma 5.2 (SLI). *Let* $\Lambda_1 \sqsubset \Lambda_2 \sqsubset \Lambda_3$. *Then we have for* $E \notin (\sigma(\mathbb{H}_{\Lambda_2}) \cup \sigma(\mathbb{H}_{\Lambda_3}))$ *the inequality*

$$\|\mathbb{1}_{\partial^i\Lambda_3} \mathbb{G}_{\Lambda_3}(E) \mathbb{1}_{\Lambda_1}\| \le \gamma \,\|\mathbb{1}_{\partial^i\Lambda_3} \mathbb{G}_{\Lambda_3}(E) \mathbb{1}_{\partial^o\Lambda_2}\|\, \|\mathbb{1}_{\partial^i\Lambda_2} \mathbb{G}_{\Lambda_2}(E) \mathbb{1}_{\Lambda_1}\|, \tag{5.9}$$

where $\gamma > 0$ *depends only on the space dimension d and the norm is the operator norm.*

Proof. The identity

$$\mathbb{H}_{\Lambda_3} = (\mathbb{H}_{\Lambda_2} \oplus \mathbb{H}_{\Lambda_3\setminus\Lambda_2}) + \mathbb{\Gamma}_{\Lambda_2} \tag{5.10}$$

and the resolvent equation imply

$$\begin{aligned}\mathbb{1}_{\partial^i\Lambda_3}\mathbb{G}_{\Lambda_3}(E)\mathbb{1}_{\Lambda_1} &= -\mathbb{1}_{\partial^i\Lambda_3}\mathbb{G}_{\Lambda_3}(E)\,\mathbb{\Gamma}_{\Lambda_2}\mathbb{G}_{\Lambda_2}(E)\mathbb{1}_{\Lambda_1}\\ &= -\mathbb{1}_{\partial^i\Lambda_3}\mathbb{G}_{\Lambda_3}(E)\mathbb{1}_{\partial^o\Lambda_2}\mathbb{\Gamma}_{\Lambda_2}\mathbb{1}_{\partial^i\Lambda_2}\mathbb{G}_{\Lambda_2}(E)\mathbb{1}_{\Lambda_1},\end{aligned} \tag{5.11}$$

where we used that $\mathbb{\Gamma}_{\Lambda_2}\mathbb{1}_{\Lambda_2} = \mathbb{1}_{\partial^o\Lambda_2}\mathbb{\Gamma}_{\Lambda_2}\mathbb{1}_{\partial^i\Lambda_2}$. Taking the norm and observing that $\gamma := \|\mathbb{\Gamma}_{\Lambda_2}\|$ depends only on the space dimension d, yields the statement. □

A similar argument proves

Lemma 5.3 (EDI). *Let Ψ be a generalized eigenfunction of $\mathbb{H}$ with generalized eigenvalue E and let γ be the constant from the previous lemma. Then we have for any Λ such that $E \notin \sigma(\mathbb{H}_\Lambda)$ and $n \in \Lambda$*

$$\|\mathbb{1}_n\Psi\| \leq \gamma\,\|\mathbb{1}_n\mathbb{G}_\Lambda(E)\mathbb{1}_{\partial^i\Lambda}\|\,\|\mathbb{1}_{\partial^o\Lambda}\Psi\|\,. \tag{5.12}$$

Proof. We infer from (5.10) with $\Lambda_3 = \mathbb{Z}^d$ and $\Lambda_2 = \Lambda$ that

$$(\mathbb{H}_\Lambda \oplus \mathbb{H}_{\mathbb{Z}^d\setminus\Lambda} - E)\Psi = -\mathbb{\Gamma}_\Lambda\Psi. \tag{5.13}$$

Since $E \notin \sigma(\mathbb{H}_\Lambda)$ and $n \in \Lambda$, this implies $\mathbb{1}_n\Psi = -\mathbb{1}_n\mathbb{G}_\Lambda(E)\mathbb{\Gamma}_\Lambda\Psi$. The identity $\mathbb{1}_\Lambda\mathbb{\Gamma}_\Lambda = \mathbb{1}_{\partial^i\Lambda}\mathbb{\Gamma}_\Lambda\mathbb{1}_{\partial^o\Lambda}$ and taking norms finishes the proof. □

The remaining part of this section is concerned with the verification of the initial-scale estimate.

Definition 5.4. Let $\theta > 0$ and $E \in \mathbb{R}$. A cube $\Lambda_L \subset \mathbb{Z}^d$, $L \in 6\mathbb{N}$, is (θ, E)-*suitable*, if $E \notin \sigma(\mathbb{H}_L)$ and

$$\|\mathbb{1}_{\partial^i\Lambda_L}\mathbb{G}_{\Lambda_L}(E)\mathbb{1}_{\Lambda_{L/3}}\| < L^{-\theta}. \tag{5.14}$$

Theorem 5.5 (Initial estimate). *Consider the random block operator $\mathbb{H}$ of Definition 1.1 and assume the hypotheses of Theorem 2.3. Then there exist constants $\theta > d$ and $p > 0$ such that for every length $L \in 6\mathbb{N}$ sufficiently large the following holds: there exists an energy $a_L > \sqrt{\lambda^2 + \beta^2}$ such that*

$$\mathbb{P}\big(\Lambda_L \textit{ is } (\theta, E)\textit{-suitable}\big) > 1 - L^{-p} \tag{5.15}$$

for every energy $E \in [-a_L, a_L]$.

We use Lifschitz tails at the internal band edges to prove Theorem 5.5. Lifschitz tails arise from a small probability for finding an eigenvalue close to the spectral edge. This mechanism also yields the high probability for the event in (5.15). As in the proof of Lifschitz tails for $\mathbb{H}$ in Section 4, we will reduce this to a corresponding statement for H.

Lemma 5.6 (Lifschitz-tail estimate [K08, Eq. (11.23)]). *Let H be the discrete random Schrödinger operator of the Anderson model as in Definition 1.1. Assume in addition that the single-site probability measure μ_V is not concentrated in a single point and let $\lambda := \inf\operatorname{supp}\mu_V$ be the infimum of the almost-sure spectrum of H. Then, given any $C, p > 0$, we have for every $L \in \mathbb{N}$ sufficiently large*

$$\mathbb{P}\big(\inf\sigma(H_L) \leq \lambda + CL^{-1/2}\big) \leq \frac{1}{L^p}. \tag{5.16}$$

As a second ingredient for the initial-scale estimate we need some natural decay of the Green function of $\mathbb{H}_L$.

Lemma 5.7 (Combes–Thomas estimate). *For $L \in \mathbb{N}$ consider the finite-volume block operator $\mathbb{H}_L$ of Definition 1.3. Fix $E \in \mathbb{R}$ with $\operatorname{dist}(E, \sigma(\mathbb{H}_L)) \geq \delta$ for some $\delta \in]0,1]$. Then we have for all $n, m \in \mathbb{Z}^d$ that*

$$\|\mathbb{1}_n \mathbb{G}_{\Lambda_L}(E)\mathbb{1}_m\| \leq \frac{4}{\delta}\, \mathrm{e}^{-(\delta/12d)\,|n-m|}\,. \tag{5.17}$$

Proof. We have patterned the lemma after [K08, Thm. 11.2], and its proof follows from a straightforward adaptation to random block operators of the proof there. Details can be found in [G11]. □

We are now ready for the

Proof of Theorem 5.5. Fix $\theta > d$, let $L \in 6\mathbb{N}$, set $a_L := \sqrt{\lambda^2 + \beta^2} + L^{-1/2}$ and pick any $E \in [-a_L, a_L]$. Assuming that the event

$$\inf \sigma(|\mathbb{H}_L|) > a_L + L^{-1/2} \tag{5.18}$$

holds, then the Combes–Thomas estimate yields

$$\|\mathbb{1}_n \mathbb{G}_{\Lambda_L}(E)\mathbb{1}_m\| \leq 4\sqrt{L}\,\mathrm{e}^{-|n-m|/(12d\sqrt{L})} \leq 4\sqrt{L}\,\mathrm{e}^{-\sqrt{L}/(48d)} \tag{5.19}$$

for all $n \in \partial^i \Lambda_L$ and all $m \in \Lambda_{L/3}$. Thus, provided L is sufficiently large, the event (5.18) implies that the cube Λ_L is (θ, E)-suitable. Negating this implication, we conclude

$$\mathbb{P}\big(\Lambda_L \text{ is not } (\theta, E)\text{-suitable}\big) \leq \mathbb{P}\big(\inf \sigma(|\mathbb{H}_L|) \leq a_L + L^{-1/2}\big). \tag{5.20}$$

The symmetry of the spectrum and the ordering (4.6) of the eigenvalues of the operators $\mathbb{H}_L$ and $\mathbb{H}_L(\beta)$ gives

$$\begin{aligned}
&\mathbb{P}\big(\Lambda_L \text{ is not } (\theta, E) \text{ -suitable}\big)\\
&\quad \leq \mathbb{P}\big(\inf \sigma(|\mathbb{H}_L(\beta)|) \leq a_L + L^{-1/2}\big)\\
&\quad \leq \mathbb{P}\Big(\inf \sigma(|\mathbb{H}_L(\beta)|) \leq \sqrt{(\lambda + CL^{-1/2})^2 + \beta^2}\Big)\\
&\quad = \mathbb{P}\big(\inf \sigma(H_L) \leq \lambda + CL^{-1/2}\big),
\end{aligned} \tag{5.21}$$

where $C \geq 1$ is some L-independent constant, and the equality in the last line relies on Lemma 4.3. The claim now follows from Lemma 5.6. □

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Magnetic Relativistic Schrödinger Operators and Imaginary-time Path Integrals

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Abstract. Three magnetic relativistic Schrödinger operators corresponding to the classical relativistic Hamiltonian symbol with magnetic vector and electric scalar potentials are considered, dependent on how to quantize the kinetic energy term $\sqrt{(\xi - A(x))^2 + m^2}$. We discuss their difference in general and their coincidence in the case of constant magnetic fields, and also study whether they are covariant under gauge transformation. Then results are reviewed on path integral representations for their respective imaginary-time relativistic Schrödinger equations, i.e., heat equations, by means of the probability path space measure related to the Lévy process concerned.

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1. Introduction

We consider the quantized operator $H := H_A + V$ corresponding to the symbol of the classical relativistic Hamiltonian

$$\sqrt{(\xi - A(x))^2 + m^2} + V(x)\,, \qquad (\xi, x) \in \mathbf{R}^d \times \mathbf{R}^d, \tag{1.1}$$

for a *relativistic* spinless particle of mass m under influence of the *magnetic* vector potential $A(x)$ and electric scalar potential $V(x)$ being, respectively, an $\mathbf{R}^d$-valued function and a real-valued function on space $\mathbf{R}^d$. This H is effectively used in the situation where one may ignore quantum-field theoretic effects like particles creation and annihilation but should take relativistic effect into consideration.

Throughout, the speed of light c and the constant $\hbar := h/2\pi$, the Planck's constant h divided by 2π, are taken to be equal to 1.

If the vector potential $A(x)$ is absent, i.e., $A(x)$ is a constant vector, we can define H as $H = H_0 + V$, where $H_0 := \sqrt{-\Delta + m^2}$ with $-\Delta$ the Laplace operator in $\mathbf{R}^d$ and V is a multiplication operator by the function $V(x)$. We can then realize not only these H_0 and V but also their sum $H_0 + V$ as selfadjoint operators in $L^2(\mathbf{R}^d)$, so long as we consider some class of reasonable scalar potential functions $V(x)$. However, when the vector potential $A(x)$ is present, the definition of H involves some sort of ambiguity. In fact, in the literature there are three kinds of quantum relativistic Hamiltonians dependent on how to quantize the kinetic energy symbol $\sqrt{(\xi - A(x))^2 + m^2}$ to get the first term H_A of H, the kinetic energy operator.

In this article, we will treat these three quantized operators $H^{(1)} = H_A^{(1)} + V$, $H^{(2)} = H_A^{(2)} + V$ and $H^{(3)} = H_A^{(3)} + V$ corresponding to the classical relativistic Hamiltonian symbol (1.1) which have the following kinetic energy parts $H_A^{(1)}$, $H_A^{(2)}$ and $H_A^{(3)}$. At first here, at least in this introduction, we assume for simplicity that $A(x)$ is a *smooth* $\mathbf{R}^d$-valued function which together with all its derivatives is bounded and that $V(x)$ is a real-valued bounded function.

The first two $H_A^{(1)}$ and $H_A^{(2)}$ are to be defined as pseudo-differential operators through oscillatory integrals. For a function f in $C_0^\infty(\mathbf{R}^d)$ put

$$(H_A^{(1)} f)(x) := \frac{1}{(2\pi)^d} \int\int_{\mathbf{R}^d \times \mathbf{R}^d} e^{i(x-y)\cdot\xi} \sqrt{\left(\xi - A\left(\frac{x+y}{2}\right)\right)^2 + m^2}\, f(y)dyd\xi, \tag{1.2}$$

$$(H_A^{(2)} f)(x) := \frac{1}{(2\pi)^d} \int\int_{\mathbf{R}^d \times \mathbf{R}^d} e^{i(x-y)\cdot\xi} \times \sqrt{\left(\xi - \int_0^1 A((1-\theta)x + \theta y)d\theta\right)^2 + m^2}\, f(y)dyd\xi. \tag{1.3}$$

The third $H_A^{(3)}$ is defined as the square root of the nonnegative selfadjoint operator $(-i\nabla - A(x))^2 + m^2$ in $L^2(\mathbf{R}^d)$:

$$H_A^{(3)} := \sqrt{(-i\nabla - A(x))^2 + m^2}. \tag{1.4}$$

$H_A^{(1)}$ is the so-called *Weyl* pseudo-differential operator defined with "mid-point prescription" treated in Ichinose–Tamura [ITa-86], Ichinose [I2-88, 3-89, 6-95]. $H_A^{(2)}$ is a modification of $H_A^{(1)}$ given by Iftimie–Măntoiu–Purice [IfMp1-07, 2-08,3-10] with their other papers. However, $H_A^{(3)}$ does not seem to be defined as a pseudo-differential operator corresponding to a certain tractable symbol. Indeed, so long as it is defined through Fourier and inverse-Fourier transforms, the candidate of its symbol will not be $\sqrt{(\xi - A(x))^2 + m^2}$ of (1.1). The last $H^{(3)}$ is used, for instance, to study "stability of matter" in relativistic quantum mechanics in Lieb–Seiringer

[LSe-10]. Needles to say, we can show that these three relativistic Schrödinger operators $H^{(1)}$, $H^{(2)}$ and $H^{(3)}$ define *selfadjoint* operators in $L^2(\mathbf{R}^d)$.

Then, letting H be one of the magnetic relativistic Schrödinger operators $H^{(1)}$, $H^{(2)}$, $H^{(3)}$ with $H_A^{(1)}$, $H_A^{(2)}$, $H_A^{(3)}$ in (1.2), (1.3), (1.4), consider the following *imaginary-time relativistic Schrödinger equation*, i.e., maybe called *heat equation* for $H - m$:

$$\frac{\partial}{\partial t}u(x,t) = -[H-m]u(x,t), \quad t > 0, \quad x \in \mathbf{R}^d. \tag{1.5}$$

The solution of the Cauchy problem with initial data $u(x,0) = g(x)$ is given by the semigroup $u(x,t) = (e^{-t[H-m]}g)(x)$. We want to deal with path integral representation for each $e^{-t[H^{(j)}-m]}g$ $(j = 1,2,3)$. The path integral concerned is connected with the *Lévy process* (e.g., [IkW2-81/89], [Sa2-99], [Ap-04/09]) on the space $D_x := D_x([0,\infty) \to \mathbf{R}^d)$ dependent on each $x \in \mathbf{R}^d$, of the *"càdlag* paths", i.e., right-continuous paths $X : [0,\infty) \ni s \mapsto X(s) \in \mathbf{R}^d$ having left-hand limits and satisfying $X(0) = x$. As our probability space (Ω, P) which is a pair of space Ω and probability P, though here and below not mentioning a σ-algebra on Ω, we take a pair (D_x, λ_x) of the path space D_x and the associated path space measure λ_x on D_x, a probability measure whose characteristic function is given by

$$e^{-t[\sqrt{\xi^2+m^2}-m]} = \int_{D_x([0,\infty)\to\mathbf{R}^d)} e^{i(X(t)-x)\cdot\xi} d\lambda_x(X), \quad t \geq 0, \quad \xi \in \mathbf{R}^d. \tag{1.6}$$

We will suppress use of the word "random variable" $\omega \in \Omega$.

The aim of this article is to make review, mainly from our results, first on some properties of these three magnetic Schrödinger operators as selfadjoint operators, for instance, that they are different in general from one another but to coincide when the vector potential $A(x)$ is linear in x, in particular, in the case of constant magnetic fields, and bounded from below by the same greatest lower bound, with study of whether they are gauge-covariant, mainly based on [I2-88, 3-89, 4-92, 8-12], [ITs1-92], [IIw-95], and next on Feyman–Kac–Itô–type path integral representations for their respective *imaginary-time* unitary groups, i.e., *real-time* semigroups mainly based on [ITa-86], [I7-95], [HILo1-12, 2-12]. It will be of some interest to collect them in one place to observe how they look like and different, though all the three are basically connected with the Lévy process.

In Section 2 we give precise definition of the three magnetic relativistic Schrödinger operators and in Section 3 more general definition, studying their properties. In Section 4 path integral representations for the semigroups for these three magnetic relativistic Schrödinger operators are given accompanied with arguments about heuristic derivation. At the end a summary is given so as to be able to compare the three path integral formulas obtained.

The content of this article is an expanded version of the lecture with almost the same title given by the author at the International Conference on "Partial Differential Equations and Spectral Theory" organized by M. Demuth, B.-W. Schulze and I. Witt, in Goslar, Germany, August 31–September 6, 2008. A brief note with condensed content on the subject with sketch of proofs also is written in [I9-12] and a rather informal introductory paper of expositary character in [I10-12]. For one of the recent references on the related subjects we refer to [LoHB-11]. I hope the present work will give a little more extensive survey to give reviews.

2. Three magnetic relativistic Schrödinger operators

In Section 1, we introduced, though rather roughly, the three magnetic relativistic Schrödinger operators $H^{(1)} = H_A^{(1)} + V$, $H^{(2)} = H_A^{(2)} + V$, $H^{(3)} = H_A^{(3)} + V$ corresponding to the classical relativistic Hamiltonian symbol (1.1). In this Section we are going to give more unambiguous definitions of them and study their properties. The difference lies in how to define their first terms on the right, kinetic energy operators $H_A^{(1)}$, $H_A^{(2)}$, $H_A^{(3)}$, corresponding to the part $\sqrt{(\xi - A(x))^2 + m^2}$ of the symbol (1.1).

2.1. Their definition and difference

For simplicity, it is assumed here as in Section 1 that the vector potential $A : \mathbf{R}^d \to \mathbf{R}^d$ is a C^∞ function and the scalar potential $V : \mathbf{R}^d \to \mathbf{R}$ is a function *bounded below*. The space of the C^∞ functions with compact support and the space of rapidly decreasing C^∞ functions in $\mathbf{R}^d$ are denoted respectively by $C_0^\infty(\mathbf{R}^d)$ and $\mathcal{S}(\mathbf{R}^d)$.

The definition of $H_A^{(1)}$, $H_A^{(2)}$ as pseudo-differential operators in (1.2), (1.3) needs the concept of *oscillatory integrals*. If the symbol $a(\eta, y)$ satisfies for some $m_0 \in \mathbf{Z}$ and $\tau_0 \geq 0$ that for any multi-indices $\alpha := (\alpha_1, \dots, \alpha_d)$, $\beta := (\beta_1, \dots, \beta_d)$ of nonnegative integers there exist constants $C_{\alpha\beta}$ such that

$$|\partial_\eta^\alpha \partial_y^\beta a(\eta, y)| \leq C_{\alpha\beta}(1 + |\eta|^2)^{m_0/2}(1 + |y|^2)^{\tau_0/2},$$

then the oscillatory integral (e.g., [Ku-74, Theorem 6.4, p. 47])

$$\text{Os-}\int\int_{\mathbf{R}^d \times \mathbf{R}^d} e^{-iy\cdot\eta} a(\eta, y)dyd\eta := \lim_{\varepsilon \to 0+} \int\int_{\mathbf{R}^d \times \mathbf{R}^d} e^{-iy\cdot\eta} \chi(\varepsilon\eta, \varepsilon y)a(\eta, y)dyd\eta \tag{2.1}$$

exists, where $\chi(\eta, y)$ is any cutoff function in $\mathcal{S}(\mathbf{R}^d \times \mathbf{R}^d)$ such that $\chi(0, 0) = 1$. The existence of the limit on the right-hand side of (2.1) is independent of the choice of cutoff functions χ, and shown by integration by parts as follows. First note that

$$(-i\partial_y)^\beta e^{-iy\cdot\eta} = (-\eta)^\beta e^{-iy\cdot\eta}, \quad (-i\partial_\eta)^\alpha e^{-iy\cdot\eta} = (-y)^\alpha e^{-iy\cdot\eta},$$

so that

$$\langle\eta\rangle^{-2l}\langle -i\partial_y\rangle^{2l} e^{-iy\cdot\eta} = e^{-iy\cdot\eta}, \quad \langle y\rangle^{-2l'}\langle -i\partial_\eta\rangle^{2l'} e^{-iy\cdot\eta} = e^{-iy\cdot\eta},$$

where

$$\langle\eta\rangle = (1 + |\eta|^2)^{1/2},\ \langle y\rangle = (1 + |y|^2)^{1/2},\ \langle -i\partial_y\rangle^2 = (1 - \Delta_y),\ \langle -i\partial_\eta\rangle^2 = (1 - \Delta_\eta).$$

Then the above note with integration by parts shows the integral before the limit $\varepsilon \to 0+$ taken is equal to

$$\begin{aligned}&\int\int e^{-iy\cdot\eta}\langle\eta\rangle^{-2l}\langle -i\partial_y\rangle^{2l}\big(\chi(\varepsilon\eta,\varepsilon y)a(\eta,y)\big)dyd\eta\\&\quad=\int\int e^{-iy\cdot\eta}\langle y\rangle^{-2l'}\langle -i\partial_\eta\rangle^{2l'}\big[\langle\eta\rangle^{-2l}\langle -i\partial_y\rangle^{2l}\big(\chi(\varepsilon\eta,\varepsilon y)a(\eta,y)\big)\big]dyd\eta\,.\end{aligned}$$

In the integral on the right above, if the positive integers l and l' are so taken that $-2l+m_0<-d$, $-2l'+\tau_0<-d$, then $\langle y\rangle^{-2l'}\langle -i\partial_\eta\rangle^{2l'}\big(\langle\eta\rangle^{-2l}\langle -i\partial_y\rangle^{2l}a(\eta,y)\big)$ becomes integrable on $\mathbf{R}^d\times\mathbf{R}^d$. Therefore taking the limit $\varepsilon\to 0+$, we see by the Lebesgue dominated convergence theorem this integral converges to

$$\int\int\langle y\rangle^{-2l'}\langle -i\partial_\eta\rangle^{2l'}\big(\langle\eta\rangle^{-2l}\langle -i\partial_y\rangle^{2l}a(\eta,y)\big)dyd\eta,$$

which implies existence of the integral Os-$\int\int e^{-iy\cdot\eta}a(\eta,y)dyd\eta$, showing existence of the oscillatory integral (2.1).

For $H_A^{(1)}$ in (1.2) we have the following proposition.

Proposition 2.1. *Let $m\geq 0$. If $A(x)$ is in $C^\infty(\mathbf{R}^d;\mathbf{R}^d)$ and satisfies for some $\tau\geq 0$ that*

$$|\partial_x^\beta A(x)|\leq C_\beta\langle x\rangle^\tau \tag{2.2}$$

for any multi-indices β with constants C_β, then for f in $C_0^\infty(\mathbf{R}^d)$ the Weyl pseudo-differential operator $H_A^{(1)}$ in (1.2) exists as an oscillatory integral and further is equal to a second expression; namely, one has

$$(H_A^{(1)}f)(x)=\frac{1}{(2\pi)^d}\text{Os–}\int\int_{\mathbf{R}^d\times\mathbf{R}^d}e^{i(x-y)\cdot\xi}\sqrt{\left(\xi-A\left(\frac{x+y}{2}\right)\right)^2+m^2}\,f(y)dyd\xi, \tag{2.3}$$

$$=\frac{1}{(2\pi)^d}\text{Os–}\int\int_{\mathbf{R}^d\times\mathbf{R}^d}e^{i(x-y)\cdot\left(\xi+A(\frac{x+y}{2})\right)}\sqrt{\xi^2+m^2}\,f(y)dyd\xi. \tag{2.4}$$

Proof. We give only a sketch of the proof, dividing into the two cases $m>0$ and $m=0$, where note that in the former case the symbol $\big((\xi-A(x))^2+m^2\big)^{1/2}$ has no singularity, but in the latter case singularity on the set $\{(\xi,x)\in\mathbf{R}^d\times\mathbf{R}^d\,;\,|\xi-A(x)|=0\}$.

(a) *The case $m>0$.* First we treat the oscillatory integral (2.3). Note that $|\partial_\xi^\alpha\partial_x^\beta\big((\xi-A(x))^2+m^2\big)^{1/2}|\leq C_{\alpha\beta}\langle\xi\rangle\langle x\rangle^\tau$, and hence $|\partial_\xi^\alpha\partial_x^\beta\big[\big((\xi-A(x))^2+m^2\big)^{1/2}f(x)\big]|\leq C_{\alpha\beta}\langle\xi\rangle\langle x\rangle^\tau$.

Since f is taken from $C_0^\infty(\mathbf{R}^d)$, we may take a cutoff function which is only dependent on the variable ξ but not y, i.e., $\chi\in\mathcal{S}(\mathbf{R}^d)$ with $\chi(0)=1$. Then we have by integration by parts as seen before this proposition,

$$
\begin{aligned}
(H_A^{(1)} f)(x) = & \lim_{\varepsilon\to 0+} \frac{1}{(2\pi)^d} \int\int_{\mathbf{R}^d\times\mathbf{R}^d} e^{i(x-y)\cdot\xi} \\
& \times \chi(\varepsilon\xi)\sqrt{\left(\xi - A\left(\frac{x+y}{2}\right)\right)^2 + m^2}\, f(y)dyd\xi \\
= & \lim_{\varepsilon\to 0+} \frac{1}{(2\pi)^d} \int\int_{\mathbf{R}^d\times\mathbf{R}^d} e^{i(x-y)\cdot\xi} \\
& \times \langle\xi\rangle^{-2l}\langle -i\partial_y\rangle^{2l}\Big(\chi(\varepsilon\xi)\sqrt{\left(\xi - A\left(\frac{x+y}{2}\right)\right)^2 + m^2}\, f(y)\Big)dyd\xi\,.
\end{aligned}
\tag{2.5}
$$

If we take l sufficiently large, $\langle\xi\rangle^{-2l}\langle -i\partial_y\rangle^{2l}\big(\sqrt{\left(\xi - A(\frac{x+y}{2})\right)^2 + m^2}\, f(y)\big)$ becomes integrable on $\mathbf{R}^d\times\mathbf{R}^d$ for fixed x, so that as $\varepsilon\to 0+$, by the Lebesgue dominated convergence theorem we have

$$
\begin{aligned}
(H_A^{(1)} f)(x) = & \frac{1}{(2\pi)^d} \int\int_{\mathbf{R}^d\times\mathbf{R}^d} e^{i(x-y)\cdot\xi} \\
& \times \langle\xi\rangle^{-2l}\langle -i\partial_y\rangle^{2l}\Big(\sqrt{\left(\xi - A\left(\frac{x+y}{2}\right)\right)^2 + m^2}\, f(y)\Big)dyd\xi\,.
\end{aligned}
\tag{2.6}
$$

This proves existence of the second oscillatory integral (2.3) for $H_A^{(1)}$ when $m>0$. Similarly, we can show existence of the second oscillatory integral (2.4). This shows the first part of the proposition.

To show the second part, i.e., coincidence of the two expressions (2.3) and (2.4), first suppose that $A(x)$ is C_0^∞. In the integral of the second member of (2.5), we make the change of variables: $\xi = \xi' + A(\frac{x+y'}{2})$, $y = y'$, where we note the Jacobian $\left|\frac{\partial(\xi,y)}{\partial(\xi',y')}\right| = 1$. Then it (= the right-hand side of (2.5)) is equal, with $\xi',\ y'$ rewritten as $\xi,\ y$ again, to

$$
\begin{aligned}
& \lim_{\varepsilon\to 0+} \int\int_{\mathbf{R}^d\times\mathbf{R}^d} e^{i(x-y)\cdot\left(\xi + A(\frac{x+y}{2})\right)} \chi\left(\varepsilon\left(\xi + A\left(\frac{x+y}{2}\right)\right)\right)\sqrt{\xi^2+m^2}\, f(y)dyd\xi \\
& = \lim_{\varepsilon\to 0+} \int\int e^{i(x-y)\cdot\xi}\langle\xi\rangle^{-2l}\langle -i\partial_y\rangle^{2l}\Big[\chi\left(\varepsilon\left(\xi + A\left(\frac{x+y}{2}\right)\right)\right) \\
& \qquad\qquad \times \sqrt{\xi^2+m^2}\, e^{i(x-y)\cdot A(\frac{x+y}{2})} f(y)\Big]dyd\xi\,,
\end{aligned}
$$

where we have integrated by parts when passing from the left-hand side to the right. Note that, since the factor $\langle\xi\rangle^{-2l}\langle -i\partial_y\rangle^{2l}\Big(\sqrt{\xi^2+m^2}\, e^{i(x-y)\cdot A(\frac{x+y}{2})} f(y)\Big)$ in the integrand on the right-hand side is integrable on $\mathbf{R}^d\times\mathbf{R}^d$ for l sufficiently large with x fixed, we can take the limit $\varepsilon\to 0+$. So the right-hand side turns out to be equal to

$$\begin{aligned}
&\int\int e^{i(x-y)\cdot\xi}\langle\xi\rangle^{-2l}\langle -i\partial_y\rangle^{2l}\Big(\sqrt{\xi^2+m^2}\, e^{i(x-y)\cdot A(\frac{x+y}{2})} f(y)\Big)dyd\xi\\
&\quad= \lim_{\varepsilon\to 0+}\int\int e^{i(x-y)\cdot\xi}\langle\xi\rangle^{-2l}\langle -i\partial_y\rangle^{2l}\Big(\chi(\varepsilon\xi)\sqrt{\xi^2+m^2}\, e^{i(x-y)\cdot A(\frac{x+y}{2})} f(y)\Big)dyd\xi\\
&\quad= \lim_{\varepsilon\to 0+}\int\int e^{i(x-y)\cdot\xi}\chi(\varepsilon\xi)\sqrt{\xi^2+m^2}\, e^{i(x-y)\cdot A(\frac{x+y}{2})} f(y)dyd\xi\\
&\quad=: \text{Os-}\int\int_{\mathbf{R}^d\times\mathbf{R}^d} e^{i(x-y)\cdot\left(\xi+A(\frac{x+y}{2})\right)}\sqrt{\xi^2+m^2}\, f(y)dyd\xi. \qquad (2.7)
\end{aligned}$$

Here the second equality is due to integration by parts. This shows coincidence of (2.3) and (2.4) for $A\in C_0^\infty(\mathbf{R}^d;\mathbf{R}^d)$.

Next, we come to the general case where $A\in C^\infty(\mathbf{R}^d;\,\mathbf{R}^d)$ satisfies (2.2). For this $A(x)$ there exists a sequence $\{A_n(x)\}_{n=1}^\infty\subset C_0^\infty(\mathbf{R}^d;\mathbf{R}^d)$ which converges to $A(x)$ in the topology of $C^\infty(\mathbf{R}^d;\,\mathbf{R}^d)$, i.e., the $A_n(x)$, together with all their derivatives, converge to $A(x)$ as $n\to\infty$ uniformly on every compact subset of $\mathbf{R}^d$. Then we have seen above the coincidence of the two expressions (2.3) and (2.4) for the Weyl pseudo-differential operators $H_{A_n}^{(1)}$ corresponding to the symbol $\big((\xi-A_n(y))^2+m^2\big)^{1/2}$. Therefore, observing (2.6) and (2.7) with A_n in place of A, we obtain

$$\begin{aligned}
&\int\int e^{i(x-y)\cdot\xi}\langle\xi\rangle^{-2l}\langle -i\partial_y\rangle^{2l}\left(\sqrt{\left(\xi-A_n\left(\frac{x+y}{2}\right)\right)^2+m^2}\, f(y)\right)dyd\xi\\
&\quad= (2\pi)^d(H_{A_n}^{(1)}f)(x)\\
&\quad= \int\int e^{i(x-y)\cdot\xi}\langle\xi\rangle^{-2l}\langle -i\partial_y\rangle^{2l}\Big(\sqrt{\xi^2+m^2}\, e^{i(x-y)\cdot A_n(\frac{x+y}{2})} f(y)\Big)dyd\xi\,.
\end{aligned}$$

Then we see with the Lebesgue convergence theorem that as $n\to\infty$, the first member and the third converge to (2.3) and (2.4), respectively, showing the coincidence of (2.3) and (2.4) in the general case.

(b) *The case* $m=0$. For our cutoff function $\chi(\xi)$, take it from $C_0^\infty(\mathbf{R}^d)$ and require further rotational symmetricity such that $0\le\chi(\xi)\le 1$ for all $\xi\in\mathbf{R}^d$ and $\chi(\xi)=1$ for $|\xi|\le\frac{1}{2}$; $=0$ for $|\xi|\ge 1$. Put $\chi_n(\xi)=\chi(\xi/n)$ for positive integer n. Then split the symbol $|\xi-A(x)|$ into a sum of two terms: $|\xi-A(x)| = h_1(\xi,x)+h_2(\xi,x)$,

$$h_1(\xi,x)=\chi_n(\xi-A(x))|\xi-A(x)|,\qquad h_2(\xi,x)=[1-\chi_n(\xi-A(x))]|\xi-A(x)|.$$

Although then the symbol $h_1(\xi,x)$ has singularity, the corresponding Weyl pseudo-differential operator can define a bounded operator on $L^2(\mathbf{R}^d)$ well, and so there is no problem. The one corresponding to the symbol $h_2(\xi,x)$, which has no more singularity, is a pseudo-differential operator defined by oscillatory integral, to which the method in the case (a) above will apply. This ends the proof of Proposition 2.1. □

For $H_A^{(2)}$ in (1.3), we can show the following proposition in the same way as Proposition 2.1.

Proposition 2.2. *Under the same hypothesis for $A(x)$ as in Proposition 2.1, for f in $C_0^\infty(\mathbf{R}^d)$ the pseudo-differential operator $H_A^{(2)}$ in (1.3) exists as an oscillatory integral and further is equal to a second expression; namely, one has*

$$(H_A^{(2)} f)(x) = \frac{1}{(2\pi)^d} \text{Os-}\int\int_{\mathbf{R}^d \times \mathbf{R}^d} e^{i(x-y)\cdot\xi} \times \sqrt{\Big(\xi - \int_0^1 A((1-\theta)x + \theta y)d\theta\Big)^2 + m^2}\, f(y)dyd\xi, \tag{2.8}$$

$$= \frac{1}{(2\pi)^d} \text{Os-}\int\int_{\mathbf{R}^d \times \mathbf{R}^d} e^{i(x-y)\cdot\big(\xi + \int_0^1 A((1-\theta)x+\theta y)d\theta\big)} \times \sqrt{\xi^2 + m^2}\, f(y)dyd\xi. \tag{2.9}$$

In the following, let us gather here, for our three magnetic relativistic Schrödinger operators $H_A^{(1)}$, $H_A^{(2)}$, $H_A^{(3)}$, all their definition for up to the present. The most general definition will be given in Section 3.

Definition 2.3. For $A \in C^\infty(\mathbf{R}^d; \mathbf{R}^d)$ satisfying condition (2.2), $H_A^{(1)}$ is defined as the pseudo-differential operators (2.3) and/or (2.4).

Definition 2.4. For $A \in C^\infty(\mathbf{R}^d; \mathbf{R}^d))$ satisfying condition (2.2), $H_A^{(2)}$ is defined as the pseudo-differential operators (2.8) and/or (2.9).

The definition of $H_A^{(3)}$ encounters a situation totally different from the previous $H_A^{(1)}$ and $H_A^{(2)}$ case. We need nonnegative selfadjointness of the operator $(-\nabla - A(x))^2$ in $L^2(\mathbf{R}^d)$, which can be considered as nothing but the nonrelativistic magnetic Schrödinger operator for a particle with mass $m = \frac{1}{2}$. Of course, if $A \in C^\infty(\mathbf{R}^d; \mathbf{R}^d)$, $(-\nabla - A(x))^2$ becomes a nonnegative, selfadjoint operator. However, more generally, it is shown by Kato and Simon (see [CFGKS, pp. 8–10]) that if $A \in L^2_{\text{loc}}(\mathbf{R}^d; \mathbf{R}^d)$, $C_0^\infty(\mathbf{R}^d)$ is a form core for the quadratic form for $(-\nabla - A(x))^2$ in $L^2(\mathbf{R}^d)$, so that by the well-known argument (e.g., [Kat-76, VI, §2, Theorems 2.1, 2.6, pp. 322–323]) there exists a unique nonnegative, selfadjoint operator in $L^2(\mathbf{R}^d)$ associated with this quadratic form with form domain $\{u \in L^2(\mathbf{R}^d)\,;\,(-\nabla - A(x))u \in L^2(\mathbf{R}^d\}$. One may take it as $(-\nabla - A(x))^2$. Then its square root $\sqrt{(-i\nabla - A(x))^2 + m^2}$ exists as a nonnegative, selfadjoint operator in $L^2(\mathbf{R}^d)$. This give the following definition for $H_A^{(3)}$.

Definition 2.5. If for $A \in L^2_{\text{loc}}(\mathbf{R}^d; \mathbf{R}^d)$, $H_A^{(3)}$ is defined as the square root:

$$H_A^{(3)} := \sqrt{(-i\nabla - A(x))^2 + m^2} \tag{2.10}$$

of the nonnegative selfadjoint operator $(-i\nabla - A(x))^2 + m^2$ in $L^2(\mathbf{R}^d)$.

We note that this $H_A^{(3)}$ does not seem to be defined as a pseudo-differential operator corresponding to a certain tractable symbol. So long as pseudo-differential operators are defined through Fourier and inverse-Fourier transforms, the candidate of its symbol will not be $\sqrt{(\xi - A(x))^2 + m^2}$. The $H_A^{(3)}$ is used, for instance, to study "stability of matter" in relativistic quantum mechanics in Lieb–Seiringer [LSei-10]. An kinetic energy inequality in the presence of the vector potential for the relativistic Schrödinger operators $H_A^{(1)}$ and $H_A^{(3)}$ as well as the nonrelativistic Schrödinger operator $(2m)^{-1}(-i\nabla - A(x))^2$ was given in [I6-93].

Needles to say, we can show that not only $H_A^{(3)}$ but also $H_A^{(1)}$ and $H_A^{(2)}$ define selfadjoint operators in $L^2(\mathbf{R}^d)$. They are in general different from one another but coincide with one another if $A(x)$ is linear in x. We observe these facts in the following.

Proposition 2.6. *$H_A^{(1)}$, $H_A^{(2)}$ and $H_A^{(3)}$ are in general different.*

Proof. First, one has $H_A^{(1)} \neq H_A^{(2)}$ for general vector potentials A, because we have

$$A\Big(\frac{x+y}{2}\Big) \neq \int_0^1 A(x + \theta(y-x))d\theta.$$

Indeed, for instance, for $d = 3$, taking $A(x) \equiv (A_1(x), A_2(x), A_3(x)) = (0, 0, x_3^2)$, we have

$$\begin{aligned}\int_0^1 A_3(x+\theta(y-x))d\theta &= \int_0^1 (x_3 + \theta(y_3 - x_3))^2 d\theta = \frac{x_3^2 + x_3y_3 + y_3^2}{3} \\ &\neq \left(\frac{x_3+y_3}{2}\right)^2 = A_3\left(\frac{x+y}{2}\right).\end{aligned}$$

Next, to see that $H_A^{(1)} \neq H_A^{(3)}$ and $H_A^{(2)} \neq H_A^{(3)}$, one needs to show (e.g., [Ho-85, Section 18.5, pp. 150–152]), for some $g \in C_0^\infty(\mathbf{R}^3)$, respectively, that

$$\begin{aligned}&\frac{1}{(2\pi)^6}\int\!\!\int\int\!\!\int e^{i(x-z)\cdot\zeta + i(z-y)\cdot\eta}\left[\left(\zeta - A\left(\frac{x+z}{2}\right)\right)^2 + m^2\right]^{1/2} \\ &\times \left[\left(\eta - A\left(\frac{z+y}{2}\right)\right)^2 + m^2\right]^{1/2} g(y)dzd\zeta dyd\eta \neq [(-\nabla - A(x))^2 + m^2]g(x),\end{aligned}$$

and that

$$\begin{aligned}&\frac{1}{(2\pi)^6}\int\!\!\int\int\!\!\int e^{i(x-z)\cdot\zeta + i(z-y)\cdot\eta}\Big[\Big(\zeta - \int_0^1 A\big(x+\theta(z-x)\big)d\theta\Big)^2 + m^2\Big]^{1/2} \\ &\times \Big[\Big(\eta - \int_0^1 A\big(z+\theta(y-z)\big)\Big)^2 + m^2\Big]^{1/2} g(y)dzd\zeta dyd\eta \neq [(-\nabla - A(x))^2 + m^2]g(x).\end{aligned}$$

Here the integrals with respect to the space variables above and below are oscillatory integrals.

The former for $H_A^{(1)}$ was shown by Umeda–Nagase [UNa-93, Section 7, p.851]. Indeed, putting $p(x,\xi) := \sqrt{(\xi - A(x))^2 + m^2}$, they verified the (Weyl) symbol $(p \circ p)(x,\xi)$ of $(H_A^{(1)})^2$ satisfy (see [UNa-93, Lemma 6.3, p. 846]; [Ho-pp.151–152]) that

$$\begin{aligned}(p \circ p)(x,\xi) &= \frac{1}{(2\pi)^6}\int\!\!\int\int\!\!\int e^{-i(y\cdot\eta + z\cdot\zeta)} p(x + \frac{z}{2}, \xi - \eta) p(x - \frac{y}{2}, \xi - \eta) dy d\eta dz d\zeta \\ &= \frac{1}{(2\pi)^6}\int\!\!\int\int\!\!\int e^{i(x-z+y/2)\cdot(\zeta-\xi)+i(z-x+y/2)\cdot(\eta-\xi)} \\ &\qquad\qquad \times p\left(\frac{x+z+y/2}{2}, \zeta\right) p\left(\frac{x+z-y/2}{2}, \eta\right) dz d\zeta dy d\eta \\ &\neq (\xi - A(x))^2 + m^2.\end{aligned}$$

The latter for $H_A^{(2)}$ will be shown in a similar way. □

Theorem 2.7. *If $A(x)$ is linear in x, i.e., if $A(x) = \dot{A} \cdot x$ with $\dot{A}$ being any $d \times d$ real symmetric constant matrix, then $H_A^{(1)}$, $H_A^{(2)}$ and $H_A^{(3)}$ coincide. In particular, this holds for constant magnetic fields with $d = 3$, i.e., when $\nabla \times A(x)$ is constant.*

Proof. Suppose $A(x) = \dot{A} \cdot x$. First, we see that $H_A^{(1)} = H_A^{(2)}$ because we have

$$\begin{aligned}\int_0^1 A(\theta x + (1-\theta)y) d\theta &= \int_0^1 \dot{A} \cdot (\theta x + (1-\theta)y) d\theta = \int_0^1 \dot{A} \cdot \big(y + \theta(x-y)\big) d\theta \\ &= \dot{A} \cdot \frac{x+y}{2} = A(\frac{x+y}{2}),\end{aligned}$$

which turns out to be "midpoint prescription" to yield the Weyl quantization.

To see that they also coincide with $H_A^{(3)}$, we need to show that $(H_A^{(1)})^2 = (-i\nabla - A(x))^2 + m^2$. To do so, let $f \in C_0^\infty(\mathbf{R}^d)$ and note $(\dot{A})^T = \dot{A}$, then we have, with integrals as oscillatory integrals,

$$\begin{aligned}\big((H_A^{(1)})^2 f\big)(x) &= \frac{1}{(2\pi)^{2d}}\int\!\!\int\int\!\!\int e^{i(x-z)\cdot(\eta + \dot{A}\frac{x+z}{2}) + i(z-y)\cdot(\xi + \dot{A}\frac{z+y}{2})} \\ &\qquad\qquad \times \sqrt{\eta^2 + m^2}\sqrt{\xi^2 + m^2} f(y) dz d\eta dy d\xi \\ &= \frac{1}{(2\pi)^{2d}}\int\!\!\int\int\!\!\int e^{iz\cdot(-\eta+\xi)} e^{i[x\cdot(\eta + \dot{A}\frac{x}{2}) - y\cdot(\xi + \dot{A}\frac{y}{2})]} \\ &\qquad\qquad \times \sqrt{\eta^2 + m^2}\sqrt{\xi^2 + m^2} f(y) dz d\eta dy \xi \\ &= \frac{1}{(2\pi)^d}\int\!\!\int\!\!\int \delta(-\eta + \xi) e^{i[x\cdot(\eta + \dot{A}\frac{x}{2}) - y\cdot(\xi + \dot{A}\frac{y}{2})]} \\ &\qquad\qquad \sqrt{\eta^2 + m^2}\sqrt{\xi^2 + m^2} f(y)\, d\eta dy d\xi\,.\end{aligned}$$

Hence

$$\begin{aligned}\big((H_A^{(1)})^2 f\big)(x) &= \frac{1}{(2\pi)^d}\int\!\!\int e^{i(x-y)\cdot\xi} e^{i\frac{1}{2}(x\cdot\dot{A}x - y\cdot\dot{A}y)}(\xi^2+m^2)f(y)\,dyd\xi \\ &= \frac{1}{(2\pi)^d}\int\!\!\int e^{i(x-y)\cdot(\xi+\dot{A}\frac{x+y}{2})}(\xi^2+m^2)f(y)\,dyd\xi \\ &= \frac{1}{(2\pi)^d}\int\!\!\int e^{i(x-y)\cdot(\xi+A(\frac{x+y}{2}))}(\xi^2+m^2)f(y)\,dyd\xi \\ &= \frac{1}{(2\pi)^d}\int\!\!\int e^{i(x-y)\cdot\xi}\big[\big(\xi-A(\frac{x+y}{2})\big)^2+m^2\big]f(y)\,dyd\xi\,.\end{aligned}$$

The last equality is due to the fact that symbol $(\xi - A(x))^2 + m^2$ is polynomial of ξ, so that the corresponding Weyl pseudo-differential operator is equal to $(-i\nabla - A(x))^2 + m^2$. □

2.2. Gauge-covariant or not

Among these three magnetic relativistic Schrödinger operators $H_A^{(1)}$, $H_A^{(2)}$ and $H_A^{(3)}$, the Weyl quantized one like $H_A^{(1)}$ (in general, the Weyl pseudo-differential operator) is *compatible well with path integral* (e.g., Mizrahi [M-78]). But the pity is that, for general vector potential $A(x)$, $H_A^{(1)}$ (and so $H^{(1)}$) is not generally covariant under gauge transformation, namely, there exists a real-valued function $\varphi(x)$ for which it fails to hold that $H_{A+\nabla\varphi}^{(1)} = e^{i\varphi}H_A^{(1)}e^{-i\varphi}$.

However, $H_A^{(2)}$ (and so $H^{(2)}$) and $H_A^{(3)}$ (and so $H^{(3)}$) are gauge-covariant, though these three are not in general equal as seen in Proposition 2.6. The gauge-covariance of the modified $H_A^{(2)}$ in contrast to $H_A^{(1)}$ in Ichinose–Tamura [ITa-86] was emphasized in Iftimie–Măntoiu–Purice [IfMP1-07, 2-08, 3-10]. There, in particular, in [IfMP1-07], they also compared our three magnetic Schrödinger operators to observe the following facts.

Proposition 2.8. *$H_A^{(2)}$ and $H_A^{(3)}$ are covariant under gauge transformation, i.e., it holds for $j = 2, 3$ that $H_{A+\nabla\varphi}^{(j)} = e^{i\varphi}H_A^{(j)}e^{-i\varphi}$ for every $\varphi \in \mathcal{S}(\mathbf{R}^d)$. But $H_A^{(1)}$ is in general not covariant under gauge transformation.*

Proof. First, to see the assertion for $H_A^{(3)} = \sqrt{(-i\nabla - A(x))^2 + m^2}$, put $K_A = (-i\nabla - A(x))^2 + m^2$, so that $H_A^{(3)} = {K_A}^{1/2}$. As $(-i\nabla - A(x))^2$ is a nonrelativistic magnetic Schrödinger operator with mass $\frac{1}{2}$, being a nonnegative selfadjoint operator on $L^2(\mathbf{R}^d)$, and gauge-covariant, so is K_A. Therefore it satisfies $K_{A+\nabla\varphi} = e^{i\varphi}K_A e^{-i\varphi}$ for every $\varphi(x)$.

It follows that $({K_{A+\nabla\varphi}}^{1/2})^2 = (e^{i\varphi}{K_A}^{1/2}e^{-i\varphi})(e^{i\varphi}{K_A}^{1/2}e^{-i\varphi})$, whence ${K_{A+\nabla\varphi}}^{1/2} = e^{i\varphi}{K_A}^{1/2}e^{-i\varphi}$, because $e^{i\varphi}{K_A}^{1/2}e^{-i\varphi}$ is also nonnegative selfadjoint.

This means that $H_{A+\nabla\varphi}^{(3)} = e^{i\varphi}H_A^{(3)}e^{-i\varphi}$, i.e., $H_A^{(3)}$ is gauge-covariant.

Next, for $H_A^{(2)}$, by the mean-value theorem

$$\varphi(y) - \varphi(x) = \int_0^1 (y-x)\cdot(\nabla\varphi)(x+\theta(y-x))d\theta$$
$$= -\int_0^1 (x-y)\cdot(\nabla\varphi)((1-\theta)x+\theta y)d\theta.$$

Hence

$$(H_A^{(2)}e^{-i\varphi}f)(x) = \frac{1}{(2\pi)^d}\int\int_{\mathbf{R}^d\times\mathbf{R}^d} e^{i(x-y)\cdot(\xi+\int_0^1 A((1-\theta)x+\theta y)d\theta)}$$
$$\times\ \sqrt{\xi^2+m^2}\, e^{-i\varphi(x)+i\int_0^1(x-y)\cdot(\nabla\varphi)((1-\theta)x+\theta y)d\theta} f(y)\, dyd\xi$$
$$= \frac{1}{(2\pi)^d}e^{-i\varphi(x)}\int\int_{\mathbf{R}^d\times\mathbf{R}^d} e^{i(x-y)\cdot(\xi+\int_0^1(A+\nabla\varphi)((1-\theta)x+\theta y)d\theta)}\sqrt{\xi^2+m^2}\, f(y)\, dyd\xi$$
$$= e^{-i\varphi(x)}(H_{A+\nabla\varphi}^{(2)}f)(x).$$

Finally, we show non-gauge-invariance of $H_A^{(1)}$. To this end, we are going to use a second expression for $H_A^{(1)}$ as an integral operator to be given in the next section, (3.7) in Definition 3.7. Then we show that it does not hold for all φ that $H_{A+\nabla\varphi}^{(1)} = e^{i\varphi}H_A^{(1)}e^{-i\varphi}$ or that, taking $A\equiv 0$. Indeed, suppose that

$$\text{p.v.}\int_{|y|>0}[e^{-iy\cdot(\nabla\varphi)(x+\frac{y}{2})}f(x+y)-f(x)]\,n(dy)$$
$$= e^{i\varphi(x)}\text{p.v.}\int_{|y|>0}[(e^{-i\varphi}f)(x+y)-(e^{-i\varphi}f)(x)]\,n(dy)$$
$$\equiv \text{p.v.}\int_{|y|>0}[e^{-i(\varphi(x+y)-\varphi(x))}f(x+y)-f(x)]\,n(dy).$$

However, the second equality cannot hold, because it does not hold for all φ that $\varphi(x+y)-\varphi(x) = y\cdot(\nabla\varphi)(x+\frac{y}{2})$. □

3. More general definition of magnetic relativistic Schrödinger operators and their selfadjointness

In this section, we want to give the most general definition of $H_A^{(1)}$, $H_A^{(2)}$ and $H_A^{(3)}$, which do *not appeal to* the pseudo-differential operators.

3.1. The most general definition of $H_A^{(1)}$, $H_A^{(2)}$ and $H_A^{(3)}$

First we concern $H_A^{(1)}$ and $H_A^{(2)}$. The starting point is the *Lévy–Khinchin formula* for the conditionally negative definite function $\sqrt{\xi^2+m^2}-m$, which has an integral representation with a σ-finite measure $n(dy)$ on $\mathbf{R}^d\setminus\{0\}$, called *Lévy measure*, which satisfies $\int_{|y|>0} \frac{|y|^2}{1+|y|^2} n(dy) < \infty$:

$$\begin{aligned}\sqrt{\xi^2+m^2}-m &= -\int_{\{|y|>0\}} [e^{iy\cdot\xi}-1-iy\cdot\xi I_{\{|y|<1\}}]n(dy) \qquad (3.1)\\ &= -\lim_{r\to 0+}\int_{|y|\geq r}[e^{iy\cdot\xi}-1]n(dy) \equiv -\text{p.v.}\int_{|y|>0}[e^{iy\cdot\xi}-1]n(dy)\,.\end{aligned}$$

Here $I_{\{|y|<1\}}$ is the indicator function of the set $\{|y|<1\}$ in $\mathbf{R}^d$, i.e., $I_{\{|y|<1\}}(z) = 1$, if $|z|<1$, and $=0$, if $|z|\geq 1$. Though the Lévy measure $n(dy)$ is m-dependent, we will suppress explicit indication of m-dependence so as to make the notation simpler. $n(dy)$ has density so that $n(dy) = n(y)dy$. The density function $n(y)$ is given by

$$n(y) = \begin{cases} 2\left(\frac{m}{2\pi}\right)^{(d+1)/2}\frac{K_{(d+1)/2}(m|y|)}{|y|^{(d+1)/2}}\,, & m>0,\\ \frac{\Gamma\left(\frac{d+1}{2}\right)}{\pi^{(d+1)/2}}\frac{1}{|y|^{d+1}}\,, & m=0,\end{cases} \qquad (3.2)$$

where $\Gamma(\tau)$ is the gamma function, and $K_\nu(\tau)$ the modified Bessel function of the third kind of order ν, which satisfies $0<K_\nu(\tau)\leq C[\tau^{-\nu}\vee\tau^{-1/2}]e^{-\tau}$, $\tau>0$ with a constant $C>0$.

To get (3.2) recall (e.g., [ITa-86, Eq. (4.2), p. 244]) the operator $e^{-t[\sqrt{-\Delta+m^2}-m]}$ has integral kernel $k_0(x-y,t)$, where

$$k_0(y,t) = \begin{cases} 2\left(\frac{m}{2\pi}\right)^{(d+1)/2}\frac{te^{mt}K_{(d+1)/2}(m(|y|^2+t^2)^{1/2})}{(|y|^2+t^2)^{(d+1)/4}}\,, & m>0,\\ \frac{\Gamma\left(\frac{d+1}{2}\right)}{\pi^{(d+1)/2}}\frac{t}{(|y|^2+t^2)^{(d+1)/2}}\,, & m=0,\end{cases} \qquad (3.3)$$

and use that fact (e.g., [IkW1-62, Example 1]) that $\frac{k_0(y,t)}{t}dy$ converges to $n(dy) = n(y)dy$, as measures on $\mathbf{R}^d$, as $t\to 0+$. Note that the both the expressions on the right-hand side of $n(y)$ in (3.2) and $k_0(y,t)$ in (3.3) are continuously connected as $m\to 0+$, because $K_\nu(\tau) = \frac{\Gamma(\nu)}{2}\left(\frac{2}{\tau}\right)^\nu(1+o(1))$ as $\tau\to 0+$.

We shall denote by $H_0\equiv\sqrt{-\Delta+m^2}$ not only the linear operator of $L^2(\mathbf{R}^d)$ into itself with domain $H^1(\mathbf{R}^d)$ but also the linear map $\mathcal{F}^{-1}\sqrt{\xi^2+m^2}\mathcal{F}$ of $\mathcal{S}'(\mathbf{R}^d)$ into itself as well as of the Sobolev space $H^s(\mathbf{R}^d)$ into $H^{s+1}(\mathbf{R}^d)$, where $\mathcal{F}$ and $\mathcal{F}^{-1}$ stand for the Fourier and inverse Fourier transforms. Now for $f\in\mathcal{S}(\mathbf{R}^d)$, put $\hat{f}=\mathcal{F}f$. The inverse Fourier transform of $\hat{f}(\xi)$ multiplied by (3.1) becomes

$$\begin{aligned}(H_0f)(x) &\equiv (\sqrt{-\Delta+m^2}f)(x) \qquad (3.4)\\ &= mf(x) - \int_{\{|y|>0\}}[f(x+y)-f(x)-I_{\{|y|<1\}}\,y\cdot\nabla_x f(x)]n(dy).\end{aligned}$$

Now to treat $H_A^{(1)}$, let $f\in C_0^\infty(\mathbf{R}^d)$ and consider, for each fixed x, the function

$$f_x:\ y\ \mapsto\ e^{i(x-y)\cdot A\left(\frac{x+y}{2}\right)}f(y),$$

which also belongs to $C_0^\infty(\mathbf{R}^d)$. Replace f in (3.4) by f_x, then we get

$$(H_0 f_x)(x) = mf(x) - \int_{\{|y|>0\}} \big[e^{-iy\cdot A(x+\frac{y}{2})} f(x+y) - f(x) - I_{\{|y|<1\}}\, y\cdot(\nabla_x - iA(x))f(x)\big] n(dy). \tag{3.5}$$

On the other hand, notice that the left-hand side of (3.5) is written by use of the Fourier transform

$$\begin{aligned}(H_0 f_x)(x) &= \frac{1}{(2\pi)^d}\text{Os–}\int\int_{\mathbf{R}^d\times\mathbf{R}^d} e^{i(x-y)\cdot\xi}\sqrt{\xi^2+m^2}\, f_x(y)dyd\xi \\ &= \frac{1}{(2\pi)^d}\text{Os–}\int\int_{\mathbf{R}^d\times\mathbf{R}^d} e^{i(x-y)\cdot\left(\xi+A(\frac{x+y}{2})\right)}\sqrt{\xi^2+m^2}\, f(y)dyd\xi\,,\end{aligned}$$

the last member of which is nothing but the second oscillatory expression (2.4) for $(H_A^{(1)}f)(x)$. Thus we have obtained the identity

$$(H_0 f_x)(x) = (H_A^{(1)}f)(x) \tag{3.6}$$

for all $f \in C_0^\infty(\mathbf{R}^d)$. This may be paraphrased "*apply* $H_A^{(1)}$ *to* f amounts to be the same thing as *apply* H_0 *to* f_x". Thus we are lead to a new definition of $H_A^{(1)}$:

$$\begin{aligned}([H_A^{(1)} - m]f)(x) :=& -\int_{|y|>0} \big[e^{-iy\cdot A(x+\frac{y}{2})} f(x+y) - f(x) \\ &\qquad - I_{\{|y|<1\}} y\cdot(\nabla_x - iA(x))\, f(x)\big] n(dy) \\ =& -\lim_{r\to 0+}\int_{|y|\ge r} \big[e^{-iy\cdot A(x+\frac{y}{2})} f(x+y) - f(x)\big]\, n(dy) \\ \equiv& -\text{p.v.}\int_{|y|>0} \big[e^{-iy\cdot A(x+\frac{y}{2})} f(x+y) - f(x)\big]\, n(dy).\end{aligned} \tag{3.7}$$

This expression makes sense for $A(x)$ being more general functions than C^∞. In fact, it can be shown with the Calderón–Zygmund theorem that the singular integral on the right-hand side of (3.7) exists pointwise in a.e. x as well as in the L^2 norm, if $A \in L^{2+\delta}_{\text{loc}}(\mathbf{R}^d; \mathbf{R}^d)$ for some $\delta > 0$ such that $\int_{0<|y|<1} |A(x+\frac{y}{2}) - A(x)||y|^{-d}dy$ is L^2_{loc}. Note that (3.7) reduces itself to (3.4) if $A(x) \equiv 0$.

For $H_A^{(2)}$, we can do it in the same way. Indeed, take $f \in C_0^\infty(\mathbf{R}^d)$ to consider, for x fixed, the function

$$f_x :\ y \mapsto e^{i(x-y)\cdot\int_0^1 A\left((1-\theta)x+\theta y\right)d\theta} f(y),$$

which belongs to $C_0^\infty(\mathbf{R}^d)$. Replacing f in (3.4) by f_x we obtain the relation $(H_0 f_x)(x) = (H_A^{(2)}f)(x)$, namely, a new definition for $H_A^{(2)}$, as follows:

$$\begin{aligned}([H_A^{(2)} - m]f)(x) :=& -\int_{|y|>0} \big[e^{-iy\cdot\int_0^1 A(x+\theta y)d\theta} f(x+y) - f(x) \\ &\qquad - I_{\{|y|<1\}} y\cdot(\nabla_x - iA(x))\, f(x)\big] n(dy)\end{aligned}$$

$$
\begin{aligned}
&:= -\lim_{r\to 0+}\int_{|y|\ge r}\left[e^{-iy\cdot\int_0^1 A(x+\theta y)d\theta} f(x+y)-f(x)\right]n(dy)\\
&\equiv -\,\text{p.v.}\int_{|y|>0}\left[e^{-iy\cdot\int_0^1 A(x+\theta y)d\theta} f(x+y)-f(x)\right]n(dy). \quad (3.8)
\end{aligned}
$$

Now we are in a position to consider the most general definition for the first two magnetic relativistic Schrödinger operators $H^{(1)} = H_A^{(1)} + V$ and $H^{(2)} = H_A^{(2)} + V$ with both general vector and scalar potentials $A(x)$ and $V(x)$. Assume that

$$A \in L^{1+\delta}_{\text{loc}}(\mathbf{R}^d) \text{ for some } \delta > 0 \text{ and } V \in L^1_{\text{loc}}(\mathbf{R}^d),\ V(x) \ge 0 \text{ a.e.}, \quad (3.9)$$

or

$$A \in L^{2+\delta}_{\text{loc}}(\mathbf{R}^d) \text{ for some } \delta > 0 \text{ and } V \in L^2_{\text{loc}}(\mathbf{R}^d),\ V(x) \ge 0 \text{ a.e.} \quad (3.10)$$

Then, first, if A and V satisfy (3.10), we can see again with the Calderón–Zygmund theorem that the singular integrals on the right-hand side of (3.7) and (3.8) exist pointwise in a.e. x as well as in the L^2 norm.

Next, if A and V satisfy (3.9), multiply (3.7) and (3.8) with $\overline{u(x)}$ and integrate them by dx, then we can reach the following quadratic forms $h^{(1)}$ and $h^{(2)}$, respectively:

$$
\begin{aligned}
h^{(1)}[u] &\equiv h^{(1)}[u,u] := h^{(1)}_{A,V}[u,u]\\
&= \Big(m\|u\|^2 + \frac{1}{2}\int\int_{|x-y|>0} |e^{-i(x-y)\cdot A(\frac{1}{2}(x+y))}u(x) - u(y)|^2 n(x-y)dxdy\Big)\\
&\qquad + \int V(x)|u(x)|^2dx =: h^{(1)}_A[u] + h^{(1)}_V[u]\,; \quad (3.11)
\end{aligned}
$$

$$
\begin{aligned}
h^{(2)}[u] &\equiv h^{(2)}[u,u] := h^{(2)}_{A,V}[u,u]\\
&= \Big(m\|u\|^2 + \frac{1}{2}\int\int_{|x-y|>0} |e^{-i(x-y)\cdot\int_0^1 A((1-\theta)x+\theta y)d\theta}u(x)\\
&\qquad\qquad - u(y)|^2 n(x-y)dxdy\Big)\\
&\qquad + \int V(x)|u(x)|^2dx =: h^{(2)}_A[u] + h^{(2)}_V[u] \quad (3.12)
\end{aligned}
$$

with form domains $Q(h^{(j)}) = \{u \in L^2(\mathbf{R}^d); h^{(j)}[u] < \infty\},\ j = 1,2$. We can see with [Kat-76, VI, §2, Theorems 2.1, 2.6, pp. 322–323] that under the assumption (3.9) for $A(x)$ and $V(x)$, there exist unique nonnegative selfadjoint operators $H^{(j)} = H_A^{(j)}\dot{+}V$ (*form sum*), $j = 1,2$, such that $h^{(j)}[u,v] = (H^{(j)}u,v)$ for $u,v \in C_0^\infty(\mathbf{R}^d)$.

We expect that the condition (3.10) (resp. (3.9)) is minimal to assure that $H^{(j)}$ (resp. $h^{(j)}$) defines a linear operator (resp. quadratic form) in $L^2(\mathbf{R}^d)$ with domain (resp. form domain) including $C_0^\infty(\mathbf{R}^d)$, so long as $V(x)$ is nonnegative. Then we can show the following results under the assumptions (3.10) and (3.9).

Theorem 3.1. ([ITs2-93]])

(i) *If* $A(x)$ *and* $V(x)$ *satisfy* (3.9), *for each* $j = 1, 2$, $h^{(j)}$ *is a closed form with form domain* $Q(h^{(j)})$ *including* $C_0^\infty(\mathbf{R}^d)$ *as a form core, so that the minimal symmetric form* $h_{\min}^{(j)}$ *defined as the form closure of* $h^{(j)}|C_0^\infty(\mathbf{R}^d) \times C_0^\infty(\mathbf{R}^d)$ *coincides with* $h^{(j)}$. *Therefore there exists a unique selfadjoint operator* $H^{(j)} = H_A^{(j)} \dot{+} V$ *(form sum) with domain* $D(H^{(j)})$ *corresponding to the form* $h^{(j)}$ *such that* $h^{(j)}[u, v] = (H^{(j)}u, v)$ *for* $u \in D(H^{(j)})$, $v \in Q(h^{(j)})$.

(ii) *If* $A(x)$ *and* $V(x)$ *satisfy* (3.10), *for each* $j = 1, 2$, $H^{(j)} = H_A^{(j)} + V$ (*operator sum*) *is essentially selfadjoint on* $C_0^\infty(\mathbf{R}^d)$ *and the closure of* $H^{(j)}$, *denoted by the same* $H^{(j)}$ *again, is bounded from below by* m.

The proof of statements in Theorem 3.1 for $H^{(1)}$ and $h^{(1)}$ were first given under less general assumption in [I3-89], [I4-93] and [ITs1-92] and completed as in the present form in [ITs2-93], while that for $H^{(2)}$ and $h^{(2)}$ given in [IfMP1-07, 2-08, 3-10] for vector potentials $A(x)$ which are C^∞ functions of polynomial growth as $|x| \to \infty$.

Thus we are led to more general definitions, not only for the two magnetic relativistic Schrödinger operators $H_A^{(1)}$ and $H_A^{(2)}$ than the ones in Definitions 2.3 and 2.4, but also for the two general relativistic Schrödinger operators $H^{(1)}$ and $H^{(2)}$ with both vector and scalar potentials $A(x)$ and $V(x)$.

Definition 3.2. If $A(x)$ and $V(x)$ satisfy (3.10), for $j = 1, 2$, $H^{(j)}$ is defined as the closure of the operator sum of the integral operator $H_A^{(j)}$ in (3.7), (3.8) and the potential $V(x)$.

Definition 3.3. If $A(x)$ and $V(x)$ satisfy (3.9), for $j = 1, 2$, $H^{(j)}$ is defined as the selfadjoint operator $H^{(j)} = H_A^{(j)} \dot{+} V$ associated with the closed form $h^{(j)}$ which is the sum of the two closed forms $h_A^{(j)}$ and $h_V^{(j)}$ as in (3.11) and (3.12).

Next, we come to $H_A^{(3)}$. If $0 < \delta < 1$, condition "$A \in L_{\text{loc}}^{1+\delta}(\mathbf{R}^d; \mathbf{R}^d)$" in (3.9) for A is slightly more general than condition "$A \in L_{\text{loc}}^2(\mathbf{R}^d; \mathbf{R}^d)$" used to give the definition for $H_A^{(3)}$ in Definition 2.5. As Theorem 3.1 (ii) says that when $A \in L_{\text{loc}}^{1+\delta}(\mathbf{R}^d; \mathbf{R}^d)$, $(-i\nabla - A(x))^2 + m^2$ can define a nonnegative selfadjoint operator in $L^2(\mathbf{R}^d)$, so we are led to the following more general definition than the one in Definition 2.5.

Definition 3.4. If $A(x)$ and $V(x)$ satisfy (3.9), $H^{(3)}$ is defined in $L^2(\mathbf{R}^d)$ as the form sum of the square root of the nonnegative selfadjoint operator $(-i\nabla - A(x))^2 + m^2$ and V:

$$H^{(3)} := H_A^{(3)} \dot{+} V := \sqrt{(-i\nabla - A(x))^2 + m^2} \dot{+} V \tag{3.13}$$

Thus, with Definitions 3.2, 3.3 and 3.4, we are now given more general definition of the three relativistic Schrödinger operators $H^{(1)}$, $H^{(2)}$, $H^{(3)}$ concerned, corresponding to the classical relativistic symbol (1.1) with both vector and scalar potentials $A(x)$ and $V(x)$.

It is appropriate here to refer, for comparison, to the corresponding results for the nonrelativistic magnetic Schrödinger operator $H^{NR} := H_A^{NR} + V := \frac{1}{2}(-i\nabla - A(x))^2 + V(x)$. In fact, as already mentioned in Section 2.1, one can realize H^{NR} as a selfadjoint operator defined through the quadratic form with form domain including $C_0^\infty(\mathbf{R}^d)$ as a form core when

$$A \in L^2_{\text{loc}}(\mathbf{R}^d) \ \text{ and } \ V \in L^1_{\text{loc}}(\mathbf{R}^d),\ V(x) \geq 0 \text{ a.e.}, \tag{3.14}$$

which was proved by Kato and Simon (see [CFKS-87, pp. 8–10]). This was also proved by Leinfelder–Simader [LeSi-81], who further gave a definitive result that it is essentially selfadjoint on $C_0^\infty(\mathbf{R}^d)$ when

$$A \in L^4_{\text{loc}}(\mathbf{R}^d),\ \text{div}A \in L^2_{\text{loc}}(\mathbf{R}^d) \ \text{ and } \ V \in L^2_{\text{loc}}(\mathbf{R}^d),\ V(x) \geq 0 \text{ a.e.} \tag{3.15}$$

The proof of Theorem 3.1 will be carried out by mimicking the arguments used by Leinfelder–Simader [LeSi-81]. First the statement (i) is proved. Then the idea of proof of the statement (ii) consists in showing that, when $A(x)$ and $V(x)$ satisfy (3.10), $C_0^\infty(\mathbf{R}^d)$ is also an operator core of the selfadjoint operator $H^{(1)}$ obtained through the form $h^{(1)}$ in the statement (i). We refer the details of the proof to Ichinose–Tsuchida [ITs2-93].

Remarks. 1°. For the scalar potential $V \in L^2_{\text{loc}}(\mathbf{R}^d)$ having negative part: $V(x) = V_+(x) - V_-(x)$ with $V_\pm(x) \geq 0$ and $V_+(x)V_-(x) = 0$ a.e., it will be possible to show the theorem, if $V_-(x)$ is small in a certain sense [i.e., relatively bounded / relatively form-bounded with respect to $\sqrt{-\Delta + m^2}$ or $H_A^{(j)}$ ($j = 1, 2$) with relative bound less than 1], but we content ourselves with such V as in (3.9) and (3.10). The main point of Theorem 3.1 is in treating the Hamiltonian with vector potential $A(x)$ as general as possible.

2°. Nagase–Umeda [NaU1-90] proved essential selfadjointness of the Weyl pseudo-differential operator $H_A^{(1)}$ in (2.3).

3°. When $A(x)$ is in $L^{2+\delta}_{\text{loc}}(\mathbf{R}^d; \mathbf{R}^d)$ and

$$\int_{0<|y|<1} |y \cdot (A(x + y/2) - A(x))||y|^{-d} dy \ \text{ is in } L^2_{\text{loc}}(\mathbf{R}^d), \tag{3.16}$$

it can be shown [ITs1-92] (cf. [I3-89]) that *Kato's inequality* holds for $H_A^{(1)}$ in (3.7): If $u \in L^2(\mathbf{R}^d)$ with $H_A^{(1)}u \in L^1_{\text{loc}}(\mathbf{R}^d)$, then the distributional inequality

$$\text{Re}((\text{sgn}\, u)[H_A^{(1)} - m]u) \geq [\sqrt{-\Delta + m^2} - m]\, |u| \tag{3.17}$$

holds, where $(\text{sgn}\, u)(x) = \overline{u(x)}/|u(x)|$ for $u(x) \neq 0$; $= 0$ for $u(x) = 0$. In particular, if $A(x)$ is Hölder-continuous, then $A(x)$ satisfies condition (3.16). To show (3.17), one has to use the expression (3.7) for $H_A^{(1)}f$ instead of (2.3). For the detail see [Its1-92, Theorem 3.1] (cf. [I3-89, Theorems 4.1, 5.1]).

In the same way, *Kato's inequality* also for $H_A^{(2)}$ will be shown with the expression (3.8) instead of (2.8): If $u \in L^2(\mathbf{R}^d)$ with $H_A^{(2)}u \in L^1_{\text{loc}}(\mathbf{R}^d)$, then the distributional inequality

$$\mathrm{Re}((\mathrm{sgn}\, u)[H_A^{(2)} - m]u) \geq [\sqrt{-\Delta + m^2} - m]\, |u| \tag{3.18}$$

holds. Also for $H_A^{(3)}$, we expect to have a distributional inequality like

$$\mathrm{Re}((\mathrm{sgn}\, u)[H_A^{(3)} - m]u) \geq [\sqrt{-\Delta + m^2} - m]\, |u|. \tag{3.19}$$

However, the problem will be open. Although it can be shown [HILo2-12] (cf. [HILo1-12]) that inequality (*Diamagnetic inequality*)

$$(f, e^{-t[H_A^{(3)} - m]} f) \leq (|f|, e^{-t[\sqrt{-\Delta+m^2} - m]} |f|) \tag{3.20}$$

holds for all $f \in L^2(\mathbf{R}^d)$, which (cf. [S1-77], [HeScUh-77]) is equivalent to an abstract version of "Kato's inequality" for $H_A^{(3)}$, the distributional version (3.20) is a stronger assertion. Here and throughout this article, $(\cdot\,, \cdot)$ in (3.20) is the *physicist's inner product* (f, g) of the Hilbert space $L^2(\mathbf{R}^d)$, which is anti-linear in f and linear in g.

Finally, we are going to see the three magnetic relativistic Schrödinger operators $H_A^{(1)}$, $H_A^{(2)}$ and $H_A^{(3)}$ are bounded from below by the *same lower bound*, as in the following theorem.

Theorem 3.5.

$$H_A^{(j)} \geq m\,, \qquad j = 1, 2, 3. \tag{3.21}$$

Proof. First, it is trivial for $H_A^{(3)}$, as also seen from (3.12), for instance. Next to see for $H_A^{(1)}$, take $u \in C_0^\infty(\mathbf{R}^d)$ in Kato's inequality (3.17) above. Multiply both sides by $|u(x)|$ and integrate them in x, then we have

$$(u, [H_A^{(1)} - m]u) \geq (|u|, [\sqrt{-\Delta + m^2} - m]\, |u|)\,,$$

where we note that $|u(x)|$ is in the Sobolev space $H^1(\mathbf{R}^d)$, so that the right-hand side above exists finite and nonnegative. So the assertion follows. In the same way it will be shown for $H_A^{(2)}$. □

Remark. In the above proof, the sharp lower bound (3.21) for $H_A^{(1)}$ and $H_A^{(2)}$ has been obtained with their integral operator expressions (3.7) and (3.8). It does not seem to be obtained by pseudo-differential calculus from their expressions (2.2)/(2.3) and (2.8)/(2.9), but instead then probably only a bound such as $H_A^{(j)} \geq m - \delta$ for some $\delta > 0$ (cf. [Ho-85, Section 18.1]).

3.2. Selfadjointness with negative scalar potentials

We have seen above that our relativistic Schrödinger operators with *nonnegative* scalar potentials assume analogous aspects on selfadjointness problem with the nonrelativistic Schrödinger operator. In this subsection we shall observe that, as for *negative* scalar potentials unbounded at infinity, the former makes a remarkable contrast with the latter, bearing an aspect closer to the Dirac operator (cf. Chernoff

[Ch-77]), though the relativistic Schrödinger equation $i\frac{\partial}{\partial t}\varphi(x,t) = [H_0 - m]\varphi(x,t)$ has not the finite propagation property.

For comparison, first we refer to the result for the nonrelativistic Schrödinger operator $-\Delta + V(x) + W(x)$ in $L^2(\mathbf{R}^d)$ by Faris–Lavine [FaLa-74] (or [RS-75, Theorem X.38, p. 198]): Assume that the real-valued scalar potentials V and W obey the following conditions: Let V be in $L^p_{\text{loc}}(\mathbf{R}^d)$ for some $p \geq (d/2) \vee 2$ ($p > 2$ when $d = 4$), and let W be in $L^2_{\text{loc}}(\mathbf{R})$ and satisfy $W(x) \geq -c_1|x|^2 - c_2$ for some constants $c_1,\ c_2$, then $-\Delta + V(x) + W(x)$ is essentially selfadjoint on $C_0^\infty(\mathbf{R}^d)$.

Now we consider the magnetic relativistic Schrödinger operator $H^{(1)} = H_A^{(1)} + V + W$, assuming the following conditions: Let A be in $L^{2+\delta}_{\text{loc}}(\mathbf{R}^d; \mathbf{R}^d)$ for some $\delta > 0$ and satisfies (3.16), and V in $L^2_{\text{loc}}(\mathbf{R}^d)$ which is relatively bounded with respect to $H_0 \equiv \sqrt{-\Delta + m^2}$ with relative bound < 1. Let W be in $L^2_{\text{loc}}(\mathbf{R}^d)$. Assume further with constants $a \geq 0,\ 0 < b \leq 1\ c \geq 0$ that

$$A(x) \text{ is bounded by a polynomial of } |x| \text{ and } W(x) \geq -c\exp[a|x|^{1-b}]\,, \tag{3.22}$$

or

$$A(x) \text{ is bounded and } W(x) \geq -ce^{a|x|}\,. \tag{3.23}$$

Note that condition (3.22) or (3.23) allows $W(x)$ to decrease exponentially at infinity with respect to $|x|^{1-b}$ or $|x|$.

Then we have the following result in [Iw-94] and [IIw-95] for the magnetic relativistic Schrödinger operator $H^{(1)} = H_A^{(1)} + V + W$. The former work used, for the operator $H_A^{(1)}$, the pseudo-differential operator expression in Definition 2.3 with (2.3), while the latter the integral operator expression connected with Lévy process in Definition 3.2 with (3.7). The latter result is sharper than the former.

Theorem 3.6. ([IIw-95]) *With the above assumption on* $A(x)$, $V(x)$ *and* $W(x)$, $H^{(1)} := H_A^{(1)} + V + W$ *is essentially selfadjoint on* $C_0^\infty(\mathbf{R}^d)$.

Example. For $0 \leq Z < (d-2)/2$, $d \geq 3$, the operator $H_A^{(1)} - Z/|x| + W(x)$ with Hölder-continuous $A(x)$ and locally square-integrable $W(x)$ satisfying (3.22) or (3.23) is essentially selfadjoint on $C_0^\infty(\mathbf{R}^d)$.

Proof of Theorem 3.6. (Sketch) First, using that V is H_0-bounded with relative bound < 1, we show that $H_A^{(1)} + V$ is a symmetric operator with domain $C_0^\infty(\mathbf{R}^d)$ bounded from below.

Next, we use Kato's inequality (3.17) for $H_A^{(1)}$ to show that if $W(x) \geq 0$ is in $L^2_{\text{loc}}(\mathbf{R}^d)$, the range of $R + H_A^{(1)} + V + W$ is dense for $R > 0$ sufficiently large, i.e., that $H_A^{(1)} + V + W$ is essentially selfadjoint on $C_0^\infty(\mathbf{R}^d)$.

Then we apply the arguments used by Faris-Lavine [FaLa-74]. The following lemma will be needed on the commutators of $H_A^{(1)}$ with the square roots of the exponential functions in (3.22) and (3.23) bounding $W(x)$ from below.

Lemma 3.7. *If* $A(x)$ *and* $V(x)$ *satisfy* (3.22) (*resp.* (3.23)), *then, for* $\psi(x) = \exp[(a/2)(1+x^2)^{(1-b)/2}]$ *with* $a \geq 0$ *and* $0 < b \leq 1$ (*resp.* $\psi(x) = \exp[(a/2)(1+$

$x^2)^{1/2}]$ *with* $0 \le a/2 < m$)*, there exists a constant* $C \ge 0$ *such that*

$$\|[H_A^{(1)}, \psi]u\| \le C\|\psi u\|, \qquad u \in C_0^\infty(\mathbf{R}^d),$$

where $[H_A^{(1)}, \psi] := H_A^{(1)}\psi - \psi H_A^{(1)}$.

The proof of Lemma 3.7 is omitted and referred to [IIw-95].

We continue the proof of Theorem 3.6. Choose a nonnegative constant K such that $K \ge 2C$ and $V(x)+ K\psi(x)^2 \ge 0$ a.e., where C and ψ are the same constant and the same function as in Lemma 3.7. Let $N = H^{(1)} + 3K\psi^2 = H_A^{(1)} + V + W + 3K\psi^2$, which is, as has been seen above, essentially selfadjoint on $C_0^\infty(\mathbf{R}^d)$. The closure of N is denoted by the same N. Then N satisfies $N \ge 2K\psi^2$ and has $C_0^\infty(\mathbf{R}^d)$ as its operator core. To prove essential selfadjointness of $H^{(1)}$ we have only to show that $\|H^{(1)}u\| \le \|Nu\|$ for $u \in C_0^\infty(\mathbf{R}^d)$ and that $\pm i[H, N] \le 3CN$ as the quadratic forms. This can be shown with the aid of the above lemma.

Finally we end the proof with the following note. When $A(x)$ and $V(x)$ satisfy (3.23), the above lemma appears to restrict the lower bound function $Ce^{a|x|}$ by $0 \le a/2 < m$, but it is not so. To see this, for the moment only here we write $H_A^{(1)}$ in (3.7) as $H_{A,m}^{(1)}$ so as to manifest its m-dependence. Then recall [I4-92, Theorem 2.3] that the difference $H_{A,m}^{(1)} - H_{A,m'}^{(1)}$ is a bounded operator for all m, $m' \ge 0$. Therefore, if it is shown that $H_{A,m}^{(1)} + V + W$ is essentially selfadjoint for some $m \ge 0$, then it follows by the Kato–Rellich theorem that so is $H_{A,m'}^{(1)} + V + W$ for every $m' \ge 0$. □

Results similar to Theorem 3.6 will hold for $H^{(2)}$ and $H^{(3)}$.

4. Imaginary-time path integrals for magnetic relativistic Schrödinger operators

It is well known that the solution $u(x,t)$ of the Cauchy problem for the heat equation $\frac{d}{dt}u(x,t) = \Big[\frac{1}{2}\Delta - V(x)\Big]u(x,t)$ with initial data $u(x,0) = g(x)$ can be represented by path integral, called *Feynman–Kac formula* (e.g., [RS-75, Theorem X.68, p. 279], [Demuth–van Casteren [DvC-00], Theorem 2.5, p. 61):

$$u(x,t) = (e^{-t[-\frac{1}{2}\Delta+V]}g)(x) = \int_{C_x([0,\infty)\to\mathbf{R}^d)} e^{-\int_0^t V(B(s))ds} g(B(t))d\mu_x(B), \quad (4.1)$$

where, for each $x \in \mathbf{R}^d$, μ_x is the *Wiener measure* on the space $C_x([0,\infty) \to \mathbf{R}^d)$ of the Brownian paths which are continuous functions $B : [0,\infty) \to \mathbf{R}^d$ satisfying $B(0) = x$. The stochastic process concerned is called *Wiener process*. As $-\frac{1}{2}\Delta+V$ is a nonrelativistic Schrödinger operator with scalar potential $V(x)$ with mass 1, so the heat equation can be thought to be *imaginary-time Schrödinger equation*, because it is the equation to be obtained by starting from (real-time) Schrödinger

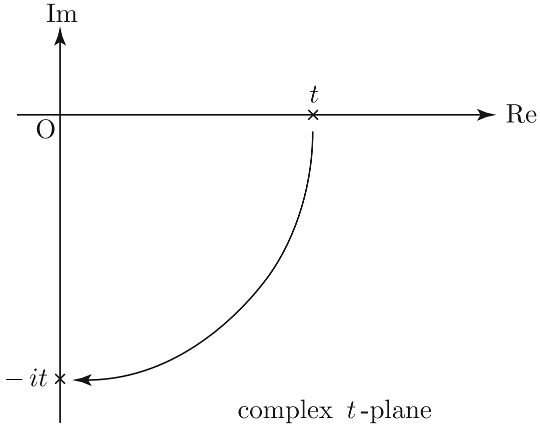

FIGURE 1. From real time t to imaginary time $-it$

equation $i\frac{\partial}{\partial t}\psi(x,t) = \Big[-\frac{1}{2}\Delta + V(x)\Big]\psi(x,t)$, next rotating it by $-90°$ from real time t to imaginary time $-it$ in complex t-plane (see Figure 1) (cf. [I5-93, Section 4, p. 23]) and then by *formally* putting $u(x,t) := \psi(x,-it)$, however, without seriously thinking about its meaning.

For a general nonrelativistic Schrödinger operator with vector and scalar potentials $A(x)$ and $V(x)$, $H^{NR} := H_A^{NR} + V := \frac{1}{2}(-i\nabla - A(x))^2 + V(x)$, there is also a path integral representation, called *Feynman–Kac–Itô formula* (e.g., Simon [S2-79/05]), for the solution $u(x,t) = (e^{-tH^{NR}}g)(x)$ of the Cauchy problem for the imaginary-time nonrelativistic Schrödinger equation, i.e., corresponding heat equation $\frac{d}{dt}u(x,t) = -H^{NR}u(x,t)$ with initial data $u(x,0) = g(x)$:

$$
\begin{aligned}
&(e^{-tH^{NR}}g)(x) \\
&\quad = \int_{C_x([0,\infty)\to\mathbf{R}^d)} e^{-[i\int_0^t A(B(s))dB(s) + \frac{i}{2}\int_0^t \operatorname{div}A(B(s))ds + \int_0^t V(B(s))ds]} g(B(t))d\mu_x(B) \\
&\quad \equiv \int_{C_x([0,\infty)\to\mathbf{R}^d)} e^{-[i\int_0^t A(B(s))\circ dB(s) + \int_0^t V(B(s))ds]} g(B(t))\,d\mu_x(B),
\end{aligned}
\tag{4.2}
$$

where $\int_0^t A(B(s))dB(s)$ is *Itô's integral* and $\int_0^t A(B(s)) \circ dB(s)$ the *Stratonovich integral*. In other words, we can say that these formulas (4.1) and (4.2) are representing the nonrelativistic Schrödinger semigroups $e^{-t[-\frac{1}{2}\Delta+V]}$ and $e^{-tH^{NR}}$.

In this section, we consider the same problem for the three magnetic relativistic relativistic Schrödinger operators $H^{(1)}$, $H^{(2)}$ and $H^{(3)}$. In Section 4.1 we give path integral representations for their respective semigroups, and in Section 4.2 we discuss how these formulas are be able to be deduced through some heuristic consideration.

4.1. Feynman–Kac–Itô type formulas for magnetic relativistic Schrödinger operators

Let H be one of the magnetic relativistic Schrödinger operators $H^{(1)}$, $H^{(2)}$, $H^{(3)}$ in Definitions 2.1, 2.2, 2.3 or Definitions 3.2, 3.3, 3.4. In the same way as in the nonrelativistic case, rotating (real-time) relativistic Schrödinger equation $i\frac{\partial}{\partial t}\psi(x,t) = [H-m]\psi(x,t)$ by $-90°$ from real time t to imaginary time $-it$ in complex t-plane (cf. [I5, Section 4, p. 23]), we arrive at the *imaginary-time relativistic Schrödinger equation*, i.e., the corresponding "heat equation" for $H-m$ [formally putting $u(x,t) := \psi(x,-it)$]:

$$\begin{cases} \dfrac{\partial}{\partial t}u(x,t) & = -[H-m]u(x,t), \quad t>0, \\ \quad u(x,0) & = g(x), \qquad\qquad\quad x \in \mathbf{R}^d. \end{cases} \tag{4.3}$$

The semigroup $u(x,t) = (e^{-t[H-m]}g)(x)$ gives the solution of this Cauchy problem as well. We want to deal with path integral representation for each $e^{-t[H^{(j)}-m]}g$ $(j=1,2,3)$. The relevant path integral is connected with the *Lévy process* (e.g., Ikeda–Watanabe [IkW2-81/89], Sato [Sa2-99], Applebaum [Ap-04/09]) on the space $D_x := D_x([0,\infty) \to \mathbf{R}^d)$, with each $x \in \mathbf{R}^d$, of the *"càdlag* paths", i.e., right-continuous paths $X : [0,\infty) \ni s \mapsto \mathbf{R}^d$ having left-hand limits and with $X(0)=x$. The associated path space measure is a probability measure λ_x, for each $x \in \mathbf{R}^d$, on $D_x([0,\infty) \to \mathbf{R}^d)$ whose characteristic function is given by

$$e^{-t[\sqrt{\xi^2+m^2}-m]} = \int_{D_x([0,\infty)\to\mathbf{R}^d)} e^{i(X(t)-x)\cdot\xi} d\lambda_x(X), \quad t \geq 0, \quad \xi \in \mathbf{R}^d. \tag{4.4}$$

This path integral formula with measure λ_x was effectively used by [CaMS-90] to get asymptotic behavior of eigenfunctions for relativistic Schrödinger operator without vector potential. It also, together with the Feyman–Kac formula (4.2) with Wiener measure μ_x, was powerfully used in [ITak1-97, 2-98] to estimate in norm the difference between the Kac transfer operator $e^{-tV/2}e^{-tH_A}e^{-tV/2}$ and the nonrelativistic and/or relativistic Schrödinger semigroup $e^{-t(H_A+V)}$ by a power of t, in the case that H_A is a nonrelativistic magnetic Schrödinger operator H_A^{NR} and/or a free relativistic Schrödinger operator $H_0 = \sqrt{-\Delta+1}-1$ with mass $m=1$.

We are going to start on task of representing the semigroup $e^{-t[H-m]}g$ by path integral. Before that, let us note that when the vector potential $A(x)$ is absent, we can represent $u(x,t)$ by a formula looking similar to the Feynman–Kac formula (4.1) for the nonrelativistic Schrödinger equation:

$$u(x,t) = (e^{-t[\sqrt{-\Delta+m^2}+V-m]}g)(x) = \int_{D_x([0,\infty)\to\mathbf{R}^d)} e^{-\int_0^t V(X(s))ds} g(X(t)) d\lambda_x(X). \tag{4.5}$$

Now, when the vector potential $A(x)$ is present, let us treat each case for $H^{(1)}$, $H^{(2)}$ and $H^{(3)}$, separately.

(1) First consider the case for $H^{(1)} := H_A^{(1)} + V$ in Definition 3.3 with condition (3.9) on $A(x)$ and $V(x)$.

To represent $e^{-t[H^{(1)}-m]}g$ by path integral, we need some further notations from Lévy process.

For each path X, $N_X(dsdy)$ denotes the *counting measure* on $[0,\infty) \times (\mathbf{R}^d \setminus \{0\})$ to count the number of discontinuities of $X(\cdot)$, i.e.,

$$N_X((t,t'] \times U) := \#\{s \in (t,t'];\, 0 \neq X(s) - X(s-) \in U\} \tag{4.6}$$

with $0 < t < t'$ and $U \subset \mathbf{R}^d \setminus \{0\}$ being a Borel set. It satisfies

$$\int_{D_x} N_X(dsdy)\, d\lambda_x(X) = dsn(dy).$$

Put

$$\widetilde{N}_X(dsdy) = N_X(dsdy) - dsn(dy), \tag{4.7}$$

which may be thought of as a renormalization of $N_X(dsdy)$. Then any path $X \in D_x([0,\infty) \to \mathbf{R}^d)$ can be expressed with $N_x(\cdot)$ and $\widetilde{N}_X(\cdot)$ as

$$\begin{aligned} X(t) - x &= \int_0^{t+} \int_{|y|\geq 1} y N_X(dsdy) + \int_0^{t+} \int_{0<|y|<1} y \widetilde{N}_X(dsdy) \\ &= \int_0^{t+} \int_{|y|>0} y \widetilde{N}_X(dsdy). \end{aligned} \tag{4.8}$$

Then we have the following path integral representation for $e^{-t[H^{(1)}-m]}g$.

Theorem 4.1. ([ITa-86], [I7-95]) *Assume that* $A(x)$ *and* $V(x)$ *satisfy condition* (3.9)*. Then*

$$(e^{-t[H^{(1)}-m]}g)(x) = \int_{D_x([0,\infty)\to\mathbf{R}^d)} e^{-S^{(1)}(X;x,t)} g(X(t))\, d\lambda_x(X), \tag{4.9}$$

$$\begin{aligned} S^{(1)}(X;x,t) &= i\int_0^{t+} \int_{|y|\geq 1} A\left(X(s-) + \frac{y}{2}\right) \cdot y\, N_X(dsdy) \\ &\quad + i\int_0^{t+} \int_{0<|y|<1} A\left(X(s-) + \frac{y}{2}\right) \cdot y\, \widetilde{N}_X(dsdy) \\ &\quad + i\int_0^{t} \int_{0<|y|<1} \left[A\left(X(s) + \frac{y}{2}\right) - A(X(s))\right] \cdot y\, dsn(dy) \\ &\quad + \int_0^t V(X(s))ds \\ &= i\int_0^{t+} \int_{|y|>0} A\left(X(s-) + \frac{y}{2}\right) \cdot y\, \widetilde{N}_X(dsdy) \qquad (4.10) \\ &\quad + i\int_0^{t} \int_{|y|>0} \left[A\left(X(s) + \frac{y}{2}\right) - A(X(s))\right] \cdot y\, dsn(dy) \\ &\quad + \int_0^t V(X(s))ds. \end{aligned}$$

Here it is easy to see the second equality in the expression (4.10) for $S^{(1)}(X;x,t)$, as well as in (4.8). We note also that, in (4.10), the integral in the third term of its second member is also written as the principal value integral:

$$\int_0^t \int_{0<|y|<1} \Big[A\Big(X(s)+\frac{y}{2}\Big) - A(X(s)\Big] \cdot y\, ds n(dy)$$
$$= \int_0^t ds\, \text{p.v.}\int_{0<|y|<1} A\Big(X(s)+\frac{y}{2}\Big) \cdot y\, n(dy),$$

and the same is valid for the second term of its third (last) member.

Proof of Theorem 4.1. We shall show first the case that both A and V are bounded and smooth, precisely, $A \in C_b^\infty(\mathbf{R}^d;\mathbf{R}^d)$ and $V \in C_b^\infty(\mathbf{R}^d;\mathbf{R})$, where, for l an positive integer, $C_b^\infty(\mathbf{R}^d;\mathbf{R}^l)$ is the Fréchet space of the $\mathbf{R}^l$-valued C^∞ functions in $\mathbf{R}^d$ which together with their derivatives of all orders are bounded. Then we shall show the general case where they satisfy condition (3.9). Our proof follows the spirit of the proof of [RS-75, Theorem X.68, p. 279] and [S2-79/05]. Representing the set Ω of "random variables ω" by the path space $D_x([0,\infty) \to \mathbf{R}^d)$, we are suppressing use of "random variable ω" by identifying it with path X.

I. The case that $A \in C_b^\infty(\mathbf{R}^d;\mathbf{R}^d)$ and $V \in C_b^\infty(\mathbf{R}^d;\mathbf{R})$.
Introduce a bounded operator $T(t)$ on $L^2(\mathbf{R}^d)$ by

$$(T(t)g)(x) := \int_{\mathbf{R}^d} k_0(x-y,t) e^{iA\left(\frac{x+y}{2}\right)\cdot(x-y)-V\left(\frac{x+y}{2}\right)t} g(y)dy$$
$$= \int_{\mathbf{R}^d} k_0(x-y,t) e^{-iA\left(\frac{x+y}{2}\right)\cdot(y-x)-V\left(\frac{x+y}{2}\right)t} g(y)dy \qquad (4.11)$$

where $k_0(x-y,t)$ is the integral kernel of $e^{-t[\sqrt{-\Delta+m^2}-m]}$ in (3.3), which is non-negative and satisfies $k_0(-x,t) = k_0(x,t)$. Then we can rewrite $T(t)$ as

$$(T(t)g)(x) = \int_{D_x} e^{-iA\left(\frac{x+X(t)}{2}\right)\cdot(X(t)-x)-V\left(\frac{x+X(t)}{2}\right)t} g(X(t)) d\lambda_x(X)\,. \qquad (4.12)$$

Do partition of $[0,t]$: $0 = t_0 < t_1 < \cdots < t_n = t,\ t_j - t_{j-1} = t/n$, and put

$$S_n(x_0,\ldots,x_n) := i\sum_{j=1}^n A\Big(\frac{x_{j-1}+x_j}{2}\Big)\cdot(x_{j-1}-x_j) + \sum_{j=1}^n V\Big(\frac{x_{j-1}+x_j}{2}\Big)\frac{t}{n}, \quad (4.13)$$

where $x_j = X(t_j)\,(j=0,1,2,\ldots,n);\ x = x_0 = X(t_0) \equiv X(0),\ y = x_n = X(t_n) \equiv X(t)$. Substitute these $n+1$ points $x_j = X(t_j)$ on the path $X(\cdot)$ into $S_n(x_0,\ldots,x_n)$ to get

$$S_n(X) := S_n(X(t_0),\ldots,X(t_n)) \qquad (4.14)$$
$$= i\sum_{j=1}^n A\Big(\frac{X(t_{j-1})+X(t_j)}{2}\Big)\cdot(X(t_{j-1})-X(t_j)) + \sum_{j=1}^n V\Big(\frac{X(t_{j-1})+X(t_j)}{2}\Big)\frac{t}{n}\,.$$

Then we have

$$\big(T(t/n)^n g\big)(x) = \overbrace{\int_{\mathbf{R}^d}\cdots\int_{\mathbf{R}^d}}^{n \text{ times}} \prod_{j=1}^{n} k_0(x_{j-1}-x_j, t/n) e^{-S_n(x_0,\dots,x_n)} g(x_n) dx_1 \cdot \dots \cdot dx_n$$
$$= \int_{D_x} e^{-S_n(X)} g(X(t))\, d\lambda_x(X), \qquad x_0 = x. \tag{4.15}$$

Before we continue further the proof of Theorem 4.1, we show the following proposition which refers to the convergence of the left-hand side of (4.15).

Proposition 4.2. *$T(t/n)^n$ converges strongly to $e^{-t[H^{(1)}-m]}$ in $L^2(\mathbf{R}^d)$ as $n \to \infty$.*

Proof. Since the operators $T(t/n)^n$ are uniformly bounded, we have only to show that $T(t/n)^n g$ is convergent to the limit in $L^2(\mathbf{R}^d)$ for g in the domain $D[H^{(1)}] = H^1(\mathbf{R}^d)$ of $H^{(1)}$. We have with $M = \sup_{x\in\mathbf{R}^d}|V(x)|$

$$\begin{aligned}
&\|T(t/n)^n g - e^{-t[H^{(1)}-m]} g\| \\
&\quad = \|\sum_{j=1}^{n} T(t/n)^{j-1}(T(t/n) - e^{-(t/n)[H^{(1)}-m]}) e^{-(n-j)(t/n)[H-m]} g\| \\
&\quad \le e^{Mt} \sup_{0\le s\le t} n\|(T(t/n) - e^{-(t/n)[H^{(1)}-m]}) e^{-s[H^{(1)}-m]} g\|,
\end{aligned}$$

which we can show tends to zero uniformly on each bounded t-interval in $[0,\infty)$ as $n \to \infty$. To see this, we show first that $(d/d\tau)(T(\tau)g)$ converges to $-[H-m]g$ in L^2, as $\tau \downarrow 0$. Indeed, we have by (3.4)

$$\begin{aligned}
&\int \big([\sqrt{-\Delta_x + m^2} - m] k_0(x-y,\tau)\big) e^{-iA\left(\frac{x+y}{2}\right)\cdot(y-x) - V\left(\frac{x+y}{2}\right)\tau} g(y) dy \\
&\quad = -\int\int_{|z|>0} [k_0(x+z-y,\tau) - k_0(x-y,\tau) - I_{\{|z|<1\}} z\cdot\nabla_x k_0(x-y,\tau)] n(dz) \\
&\qquad\qquad \times e^{-iA\left(\frac{x+y}{2}\right)\cdot(y-x) - V\left(\frac{x+y}{2}\right)\tau} g(y) dy \\
&\quad = -\int\int_{|z|>0} \Big[k_0(x-y,\tau) e^{-iA\left(\frac{x+z+y}{2}\right)\cdot(z+y-x) - V\left(\frac{x+z+y}{2}\right)\tau} g(z+y) \\
&\qquad\qquad - \Big(k_0(x-y,\tau) - I_{\{|z|<1\}} z\cdot\nabla_x k_0(x-y,\tau)\Big) \\
&\qquad\qquad\qquad \times e^{-iA\left(\frac{x+y}{2}\right)\cdot(y-x) - V\left(\frac{x+y}{2}\right)\tau} g(y)\Big] n(dz) dy,
\end{aligned}$$

where we have changed the variable $z - y =: -y'$ and then rewritten y for y' again. Then noting that $\nabla_x k_0(x-y,\tau) = -\nabla_y k_0(x-y,\tau)$ and integrating by parts in the variable y, we see that the above integral converges to

$$-\int_{|z|>0} [e^{-iz\cdot A\left(x+\frac{z}{2}\right)} g(x+z) - g(x) - I_{\{|z|<1\}} z\cdot\nabla_x g(x)] n(dz),$$

as $\tau \to +0$, because then $k_0(x-y,\tau) \to \delta(x-y)$. It follows that, as $\tau \to +0$,

$$\left(\frac{\partial}{\partial\tau}T(\tau)g\right)(x) = -\int_{|y|>0}\Big[\Big(\big[\sqrt{-\Delta_x+m^2}-m\big]+V(\frac{x+y}{2}\Big)k_0(x-y,\tau)\Big] \times e^{-iA\left(\frac{x+y}{2}\right)\cdot(y-x)-V\left(\frac{x+y}{2}\right)\tau}g(y)dy$$

converges to

$$-\int_{|z|>0}\big[e^{-iA\left(x+\frac{z}{2}\right)\cdot z}g(x+z)-g(x)-I_{|z|<1}z\cdot\nabla_x g(x)\big]n(dz)-V(x)g(x) = (-[H^{(1)}-m]g)(x).$$

Thus we see that for $h \in D[H^{(1)}]$

$$\begin{aligned} &n\|[T(t/n)-e^{-(t/n)[H^{(1)}-m]}]h\| \\ &= n\Big\|\int_0^{t/n}\frac{\partial}{\partial\tau}\big[T(\tau)-e^{-\tau[H^{(1)}-m]}\big]hd\tau\Big\| \\ &= n\Big\|\int_0^{t/n}\Big(\frac{\partial}{\partial\tau}T(\tau)+[H^{(1)}-m]e^{-\tau[H^{(1)}-m]}\Big)hd\tau\Big\| \\ &\le t\sup_{0\le\tau\le t/n}\Big\|\Big(\frac{\partial}{\partial\tau}T(\tau)+[H^{(1)}-m]e^{-\tau[H^{(1)}-m]}\Big)h\Big\| \end{aligned}$$

converges to zero as $n \to \infty$. Moreover, this convergence is uniform on compact subsets in $t \ge 0$ as $n \to \infty$. Noting $D[H^{(1)}]$ is a Hilbert space $D[H^{(1)}]$ with graph norm of $H^{(1)}-m$, we see by uniform boundedness principle that the sequence $\{n\big(T(t/n)-e^{-(t/n)[H^{(1)}-m]}\big)\}_{n=1}^{\infty}$ is, as a family of bounded operators of the Hilbert space $D[H^{(1)}]$ into $L^2(\mathbf{R}^d)$, uniformly bounded for all n and on every fixed compact subset in $t \ge 0$. Consequently, it converges to zero uniformly on compact subsets of the Hilbert space $D[H^{(1)}]$. The map $[0,t] \ni s \mapsto e^{-s[H^{(1)}-m]} \in D[H^{(1)}]$ is continuous, so that $\{e^{-s[H^{(1)}-m]}g;\, 0 \le s \le t\}$ is a compact subset of $D[H^{(1)}]$. This shows Proposition 4.2. □

We continue the proof of Theorem 4.1, I.

To see the convergence of the right-hand side of (4.15), put

$$S_n(X) = S_{n1}(X)+S_{n2}(X), \tag{4.16}$$

$$S_{n1}(X) = i\sum_{j=1}^{n}A\Big(\frac{X(t_{j-1})+X(t_j)}{2}\Big)\cdot(X(t_j)-X(t_{j-1})), \tag{4.17}$$

$$S_{n2}(X) = \sum_{j=1}^{n}V\Big(\frac{X(t_{j-1})+X(t_j)}{2}\Big)(t_j-t_{j-1}). \tag{4.18}$$

First, for $S_{n2}(X)$ in (4.18), it is evident that for each $X \in D_x$, $S_{n2}(X)$ converges to $\int_0^t V(X(s))ds$, i.e., the last term of the second member of (4.10), as $n \to \infty$.

Next, to see the convergence of $S_{n1}(X)$ in (4.17) to the sum of the other three terms in the same (second) member of (4.10) which involve $A(\cdot)$, we rewrite by Itô's formula [IkW2-81/89, Chap. II, 5, Theorem 5.1] (cf. (4.8)) the summand in $S_{n1}(X)$ as

$$
\begin{aligned}
&A\Big(\frac{X(t_{j-1})+X(t_j)}{2}\Big)\cdot(X(t_j)-X(t_{j-1}))\\
&=\int_{t_j-1}^{t_j+}\int_{|y|>0}\Big[A\Big(\frac{X(s-)+X(t_{j-1})+yI_{|y|\ge 1}(y)}{2}\Big)\\
&\qquad\qquad \times\big(X(s-)-X(t_{j-1})+yI_{\{|y|\ge 1\}}(y)\big)\\
&\qquad\qquad - A\Big(\frac{X(s-)+X(t_{j-1})}{2}\Big)\cdot\big(X(s-)-X(t_{j-1})\big)\Big]\,N_X(dsdy)\\
&+\int_{t_j-1}^{t_j+}\int_{|y|>0}\Big[A\Big(\frac{X(s-)+X(t_{j-1})+yI_{|y|<1}(y)}{2}\Big)\\
&\qquad\qquad \times\big(X(s-)-X(t_{j-1})+yI_{\{|y|<1\}}(y)\big)\\
&\qquad\qquad - A\Big(\frac{X(s-)+X(t_{j-1})}{2}\Big)\cdot\big(X(s-)-X(t_{j-1})\big)\Big]\,\widetilde{N}_X(dsdy)\\
&+\int_{t_j-1}^{t_j}\int_{|y|>0}\Big\{A\Big(\frac{X(s)+X(t_{j-1})+yI_{|y|<1}(y)}{2}\Big)\\
&\qquad\qquad \times\big(X(s)-X(t_{j-1})+yI_{\{|y|<1\}}(y)\big)\\
&\qquad\qquad - A\Big(\frac{X(s)+X(t_{j-1})}{2}\Big)\cdot\big(X(s)-X(t_{j-1})\big)\\
&\qquad\qquad - I_{\{|y|<1\}}(y)\Big[\Big(\frac{1}{2}(y\cdot\nabla)A\Big)\Big(\frac{X(s)+X(t_{j-1}}{2}\Big)\cdot\big(X(s)-X(t_{j-1})\big)\\
&\qquad\qquad + y\cdot A\Big(\frac{X(s)+X(t_{j-1})}{2}\Big)\Big]\Big\}\,dsn(dy).
\end{aligned}
$$

Then, taking $n=2^k$ so that $t_j=2^{-k}jt$, $j=0,1,\dots,2^k$, we can see for each $X\in D_x$ that as $k\to\infty$, $S_{n1}(X)$ converges to the sum of the first, second and third terms in the second member of (4.10). Thus $S_n(X)$ in (4.14)/(4.16) converges to the second member of (4.10), therefore $S^{(1)}(X;x,t)$. As a result, by the Lebesgue dominated convergence theorem the right-hand side of (4.15) converges to the right-hand side of (4.9).

II. The general case where $A(x)$ and $V(x)$ satisfy condition (3.9).

Choose a sequence $\{A_k\}$ in $C_b^\infty(\mathbf{R}^d;\mathbf{R}^d)$ with $|A_k(x)|\le|A(x)|$ which is convergent to $A(x)$ in $L^{1+\delta}_{\mathrm{loc}}$ and pointwise a.e., and a sequence $\{V_k\}$ in $C_b^\infty(\mathbf{R}^d;\mathbf{R})$ with $0\le V_k(x)\le V(x)$ which is convergent to $V(x)$ in L^1_{loc} and pointwise a.e., as $k\to\infty$. Then by (4.9), (4.10) we have

$$(e^{-t[H_k^{(1)}-m]}g)(x)=\int_{D_x}e^{-S_k(X;x,t)}g(X(t))d\lambda_x(X), \tag{4.19}$$

where $S_k(X;x,t)$ (though here with superscript $^{(1)}$ removed, for notational simplicity) is the $S^{(1)}(X;x,t)$ in (4.10) with A_k and V_k in place of A and V, and $H_k^{(1)}$ is the selfadjoint operator associated with the form $h_k^{(1)} \equiv h_{A_k,V_k}^{(1)}$ in (2.5). We shall show both sides of (4.19) converge to those of (4.9) as $k \to \infty$.

As far as the left-hand side of (4.19) is concerned, by [ITs2-93, Lemma 3.6], $H_k^{(1)}$ converges to $H^{(1)}$ in the strong resolvent sense, and by [Kat-76, IX, Theorem 2.16, p.504], $\{\exp[-t(H_k^{(1)}-m)]g\}_{k=1}^{\infty}$ converges to $\exp[-t(H^{(1)}-m)]g$, uniformly on each bounded t-interval in $[0,\infty)$, in L^2 and, if a subsequence is taken, pointwise a.e.

To see convergence of the right-hand side of (4.19), we shall show that $\{\exp[-S_k(X;x,t)]\}_{k=1}^{\infty}$ converges for a.e. x and λ_x-a.e. X, as $k \to \infty$, and its limit can be written as $e^{-S^{(1)}(X;x,t)}$. Put

$$S_k(X;x,t) = \sum_{j=1}^{4} S_k^{\langle j\rangle}(X;x,t), \qquad S^{(1)}(x,t) = \sum_{j=1}^{4} S^{\langle j\rangle}(X;x,t).$$

We show each $\exp[-S_k^{\langle j\rangle}(X;x,t)]$ $(j=1,2,3,4)$ converges for λ_x-a.e. X.

(i) There exists a Borel set K_1 in $\mathbf{R}^d$ of Lebesgue measure zero such that $|A(x)|$ is finite and $A_k(x) \to A(x)$ for $x \notin K_1$. Then for each (s,y) with $0 < s \le t$ and $|y| \ge 1$,

$$G_1(s,y) := \{X \in D_x;\ X(s-) + y/2 \in K_1\}$$

has λ_x-measure zero, because

$$\int_{G(s,y)} d\lambda_x(X) = \int_{K_1 - y/2} k_0(s, x-z)dz = 0.$$

Therefore by the Fubini theorem

$$G_1 := \{(X,s,y) \in D_x \times (0,t] \times \{|y| \ge 1\};\ X(s-) + y/2 \in K_1\}$$

has $[d\lambda_x \times dsn(dy)]$-measure zero, because

$$\int\int\int I_{G_1}(X,s,y)d\lambda_x dsn(dy) = \int_0^t \int_{|y|\ge 1} dsn(dy) \int_{G_1(s,y)} d\lambda_x(X) = 0,$$

where $I_{G_1}(X,s,y)$ is the indicator function for the set G_1. It follows again by the Fubini theorem that for λ_x-a.e. X,

$$G_1(X) := \{(s,y) \in (0,t] \times \{|y| \ge 1\};\ X(s-) + y/2 \in K_1\}$$

has $N_X(dsdy)$-measure zero, since

$$\int_{D_x} d\lambda_x(X) \int\int_{G_1(X)} N_X(dsdy) = \int_{D_x} d\lambda_x(X) \int\int_{G_1(X)} dsn(dy).$$

Therefore for λ_x-a.e. X, as $k \to \infty$,

$$A_k(X(s-) + y/2) \to A(X(s-) + y/2), \qquad N_X(dsdy) - \text{a.e.},$$

and the integral $S_k^{\langle 1\rangle}(X;x,t)$ exists, being a finite sum because $X(s)$ has at most finitely many discontinuities s with the jump $|X(s)-X(s-)|$ exceeding a given positive constant. By the Lebesgue dominated convergence theorem, for λ_x-a.e. X, $S_k^{\langle 1\rangle}(X;x,t) \to S^{\langle 1\rangle}(X;x,t)$ and hence $\exp[-S_k^{\langle 1\rangle}(X;x,t)] \to \exp[-S^{\langle 1\rangle}(X;x,t)]$.

(ii) For $n>0$ let $\sigma_n(X)=\inf\{s>0;\ |X(s-)|>n\}$. Then for λ_x-a.e. X, $\lim_{n\to\infty}\sigma_n(X)=\infty$. For k, l integers put $A_{kl}(x)=A_k(x)-A_l(x)$, and

$$G_2^{kl} := \{(X,s,y)\in D_x\times(0,t]\times\{0<|y|<1\};\ |A_{kl}(X(s-)+y/2)\cdot y|>1\}$$

and for each $X\in D_x$

$$G_2^{kl}(X) := \{(s,y)\in(0,t]\times\{0<|y|<1\};\ |A_{kl}(X(s-)+y/2)\cdot y|>1\}.$$

The complements of G_2^{kl} in the set $D_x\times(0,t]\times\{0<|y|<1\}$ and $G_2^{kl}(X)$ in the set $(0,t]\times\{0<|y|<1\}$ are denoted by $(G_2^{kl})^c$ and $(G_2^{kl}(X))^c$, respectively. Then we have, for n fixed and for an arbitrary compact subset K of $\mathbf{R}^d$ with Lebesgue measure $|K|$,

$$\begin{aligned}
&\int_K dx\int_{D_x}|S_k^{\langle 2\rangle}(X;x,t\wedge\sigma_n(X)) - S_l^{\langle 2\rangle}(X;x,t\wedge\sigma_n(X))|d\lambda_x(X)\\
&\le \int_K dx\int_{D_x}\Big|\int\int_{G_2^{kl}(X)} I_{[0,\sigma_n(X)]}(s)A_{kl}(X(s-)+y/2)\cdot y\widetilde{N}_X(dsdy)\Big|d\lambda_x(X)\\
&\quad+\int_K dx\int_{D_x}|\int\int_{(G_2^{kl}(X))^c} I_{[0,\sigma_n(X)]}(s)A_{kl}(X(s-)+y/2)\cdot y\widetilde{N}_X(dsdy)|d\lambda_x(X)\\
&\equiv \int_K I_1^{kl}dx + \int_K I_2^{kl}dx.
\end{aligned}$$

For I_1^{kl} we have

$$\begin{aligned}
\int_K I_1^{kl}dx &\le \int_K dx\int_{D_x}d\lambda_x(X)\\
&\qquad\times\int\int_{G_2^{kl}(X)} I_{[0,\sigma_n(X)]}(s)|A_{kl}(X(s-)+y/2)\cdot y|(N_X(dsdy)+dsn(dy))\\
&\le 2\int_K dx\int_{D_x}d\lambda_x(X)\int\int_{G_2^{kl}(X)} I_{[0,\sigma_n(X)]}(s)|A_{kl}(X(s)+y/2)\cdot y|^{1+\delta}dsn(dy)\\
&\le 2\int dx\int_0^t\int_{0<|y|<1}dsn(dy)\int_{|z|\le n}|A_{kl}(z+y/2)\cdot y|^{1+\delta}k_0(s,x-z)dz\\
&\le 2n_\delta t\int_{|z|\le n+1}|A_{kl}(z)|^{1+\delta}dz,
\end{aligned}$$

with $n_\delta=\int_{0<|y|<1}|y|^{1+\delta}n(dy)$, where in the second inequality we have used that $|A_{kl}(X(s)+y/2)\cdot y|>1$ on $G_2^{kl}(X)$.

For I_2^{kl} we have

$$\begin{aligned}(I_2^{kl})^2 &= \int_{D_x} d\lambda_x(X) \int\int_{(G_2^{kl}(X))^c} I_{[0,\sigma_n(X)]}(s)|A_{kl}(X(s)+y/2)\cdot y|^2 dsn(dy) \\ &\le \int_{D_x} d\lambda_x(X) \int\int_{(G_2^{kl}(X))^c} I_{[0,\sigma_n(X)]}(s)|A_{kl}(X(s)+y/2)\cdot y|^{1+\delta} dsn(dy) \\ &= \int_0^t \int_{0<|y|<1} dsn(dy) \int_{|z|\le n} |A_{kl}(z+y/2)\cdot y|^{1+\delta} k_0(s,x-z)dz,\end{aligned}$$

where the inequality is due to that $|A_{kl}(X(s)+y/2)\cdot y| \le 1$ on $(G_2^{kl}(X))^c$. Hence

$$\begin{aligned}\int_K I_2^{kl} dx &\le |K|^{1/2}\left(\int (I_2^{kl})^2 dx\right)^{1/2} \\ &= |K|^{1/2}\bigg(\int dx \int_0^t \int_{0<|y|<1} dsn(dy) \\ &\qquad \times \int_{|z|\le n} |A_{kl}(z+y/2)\cdot y|^{1+\delta} k_0(s,x-z)dz\bigg)^{1/2} \\ &\le (|K|n_\delta t)^{1/2}\left(\int_{|z|\le n+1} |A_{kl}(z)|^{1+\delta} dz\right)^{1/2}.\end{aligned}$$

Thus we have

$$\begin{aligned}&\int_K dx \int_{D_x} |S_k^{\langle 2\rangle}(X;x,t\wedge\sigma_n(X)) - S_l^{\langle 2\rangle}(X;x,t\wedge\sigma_n(X))| d\lambda_x(X) \\ &\quad\le \int_K I_1^{kl} dx + \int_K I_2^{kl} dx \\ &\quad\le 2n_\delta t \int_{|z|\le n+1} |A_{kl}(z)|^{1+\delta} dz + (|K|n_\delta t)^{1/2}\left(\int_{|z|\le n+1} |A_{kl}(z)|^{1+\delta} dz\right)^{1/2},\end{aligned}$$

which tends to zero as $k, l \to \infty$. Since K is arbitrary, it can be seen, by passing to a subsequence, for a.e. x, that as $k \to \infty$, $\{S_k^{\langle 2\rangle}(X;x,t\wedge\sigma_n(X))\}_{k=1}^\infty$ converges to a limit in L^1 with respect to λ_x and, by passing to a subsequence, for λ_x-a.e. X. This limit is what is to be denoted by $S^{\langle 2\rangle}(X;x,t\wedge\sigma_n(X))$. Further, since $\lim_{n\to\infty}\sigma_n(X) = \infty$ for λ_x-a.e. X, we see that $\{S_k^{\langle 2\rangle}(X;x,t)\}_{k=1}^\infty$ converges to a limit for λ_x-a.e. X, which is to be denoted by $S^{\langle 2\rangle}(X;x,t)$, and hence $\exp[-S_k^{\langle 2\rangle}(X;x,t)] \to \exp[-S^{\langle 2\rangle}(X;x,t)]$.

(iii) We can show with the theory of singular integrals that

$$a(x) := \text{p.v.}\int_{0<|y|<1} A(x+y/2)\cdot y\, n(dy)$$

exists pointwise a.e. in x, while

$$a_k(x) := \int_{0<|y|<1} (A_k(x+y/2)-A_k(x))\cdot y\, n(dy) = \text{p.v.}\int_{0<|y|<1} A_k(x+y/2)\cdot y\, n(dy)$$

exists for every x, and that as $k \to \infty$, $a_k(x)$ converges to $a(x)$ in $L^{1+\delta}_{\rm loc}$. With the same $\sigma_n(X)$ as in (ii), we have, for n fixed,

$$\begin{aligned}
&\int_{\mathbf{R}^d} dx \int_{D_x} |S_k^{\langle 3\rangle}(X;x,t\wedge\sigma_n(X)) - S_l^{\langle 3\rangle}(X;x,t\wedge\sigma_n(X))|^{1+\delta} d\lambda_x(X)\\
&\quad = \int dx \int d\lambda_x(X) \Big| \int_0^t I_{[0,\sigma_n(X)]}(s)[a_k(X(s)) - a_l(X(s))]ds \Big|^{1+\delta}\\
&\quad \le \int dx \int d\lambda_x(X) \Big(\int_0^t ds \Big)^{\delta} \int_0^t I_{[0,\sigma_n(X)]}(s) |a_k(X(s)) - a_l(X(s))|^{1+\delta} ds\\
&\quad \le t^{\delta} \int dx \int_0^t ds \int_{|z|\le n} |(a_k(z) - a_l(z))|^{1+\delta} k_0(s, x-z) dz\\
&\quad \le t^{1+\delta} \int_{|x|\le n} |(a_k(x) - a_l(x)|^{1+\delta} dx \to 0, \qquad k,l\to\infty,
\end{aligned}$$

where in the first inequality we have used the Hölder inequality. Similarly to (ii), it can be seen, by passing to a subsequence, for a.e. x, that as $k \to \infty$, $\{S_k^{\langle 3\rangle}(X;x,t\wedge\sigma_n(X))\}_{k=1}^{\infty}$ converges to a limit in $L^{1+\delta}$ with respect to λ_x and, by passing to a subsequence, for λ_x-a.e. X. This limit is what is to be denoted by $S^{\langle 3\rangle}(X;x,t\wedge\sigma_n(X))$. Further, since $\lim_{n\to\infty}\sigma_n(X) = \infty$ for λ_x-a.e. X, we see that $\{S_k^{\langle 3\rangle}(X;x,t)\}_{k=1}^{\infty}$ converges to a limit for λ_x-a.e. X, which is to be denoted by $S^{\langle 3\rangle}(X;x,t)$, and hence $\exp[-S_k^{\langle 3\rangle}(X;x,t)] \to \exp[-S^{\langle 3\rangle}(X;x,t)]$.

(iv) The proof will proceed in the same way as the proof of [S2-79/05, II, Theorem 6.2, p. 51]. We may suppose that $V_k(x) \uparrow V(x)$ pointwise a.e. There exists a Borel set K_4 in $\mathbf{R}^d$ of Lebesgue measure zero such that $V_n(x) \uparrow V(x)$ for $x \notin K_4$. Then for $0 < s \le t$,

$$G_4(s,y) = \{X \in D_x;\ X(s) \in K_4\}$$

has λ_x-measure zero. Therefore by the Fubini theorem

$$G_4 = \{(X,s) \in D_x \times (0,t];\ X(s) \in K_4\}$$

has $[d\lambda_x \times ds]$-measure zero, so that for λ_x-a.e. X,

$$G_4(X) = \{s \in (0,t];\ X(s) \in K_4\}$$

has Lebesgue measure zero. It follows by the monotone convergence theorem that for λ_x-a.e. X, $S_n^{\langle 4\rangle}(X;x,t) \to S^{\langle 4\rangle}(X;x,t)$ and hence $\exp[-S_n^{\langle 4\rangle}(X;x,t)] \to \exp[-S^{\langle 4\rangle}(X;x,t)]$. This proves Theorem 4.1. □

(2) Next we come to the case for $H^{(2)} := H_A^{(2)} + V$ in Definition 3.3 with condition (3.9) on $A(x)$ and $V(x)$.

Theorem 4.3. [IfMP1-07, 2-08, 3-10] *The same hypothesis as in Theorem* 4.1.

$$(e^{-t[H^{(2)}-m]}g)(x) = \int_{D_x([0,\infty)\to\mathbf{R}^d)} e^{-S^{(2)}(X;x,t)}g(X(t))\,d\lambda_x(X), \tag{4.20}$$

$$\begin{aligned} S^{(2)}(X;x,t) &= i\int_0^{t+}\int_{|y|>0}\Big(\int_0^1 A(X(s-)+\theta y)d\theta\Big)\cdot y\,\widetilde{N}_X(dsdy) \qquad (4.21)\\ &\quad + i\int_0^t\int_{|y|>0}\Big[\int_0^1 A(X(s)+\theta y)d\theta - A(X(s))\Big]\cdot ydsn(dy)\\ &\quad + \int_0^t V(X(s))ds. \end{aligned}$$

The proof of Theorem 4.3 can be done in exactly the same way as that of Theorem 4.1. Indeed, we have only to replace $A(X(s-)+\frac{y}{2})\cdot y$ by $(\int_0^1 A(X(s-)+\theta y)d\theta)\cdot y$. We will not repeat it here.

(3) Finally, we consider the case for the operator defined, in Definition 3.4, with the square root of a nonnegative selfadjoint operator, $H^{(3)} := H_A^{(3)} + V$.

On the one hand, we can determine by functional analysis, namely, by theory of fractional powers (e.g., Yosida [Y, Chap. IX, 11, pp. 259–261]) $e^{-t[H_A^{(3)}-m]}$ from the nonnegative selfadjoint operator $S := (-i\nabla - A(x))^2 + m^2 =: 2H_A^{NR,1} + m^2$ where H_A^{NR} stands for the magnetic nonrelativistic Schrödinger operator $\frac{1}{2}(-i\nabla - A(x))^2$ with mass 1 without scalar potential. Indeed, we have

$$e^{-t[H_A^{(3)}-m]}g = \begin{cases} e^{mt}\int_0^\infty f_t(\kappa)e^{-\kappa S}g\,d\kappa, & t>0,\\ 0, & t=0\end{cases}$$

$$f_t(\kappa) = \begin{cases} (2\pi i)^{-1}\int_{\sigma-i\infty}^{\sigma+i\infty} e^{z\kappa - tz^{1/2}}dz, & \kappa\ge 0,\\ 0, & \kappa<0 \quad (\sigma>0).\end{cases} \tag{4.22}$$

This equation (4.22) may provide a kind of path integral representation for $e^{-t[H_A^{(3)}-m]}g$ with the Wiener measure μ_x:

$$\begin{aligned} &(e^{-t[H_A^{(3)}-m]}g)(x)\\ &\quad = e^{mt}\int_0^\infty d\kappa\, f_t(\kappa)e^{-\kappa m^2}\\ &\qquad \times \int_{C_x([0,\infty)\to\mathbf{R}^d)} e^{-[i\int_0^{2\kappa} A(B(s))\circ dB(s) + \int_0^{2\kappa} V(B(s))ds]}g(B(2\kappa m))\,d\mu_x(B), \end{aligned}$$

though with an undesirable extra $d\kappa$-integral, by substituting the Feynman–Kac–Itô formula (4.2) with $V=0$, i.e., for $e^{-t[H_A^{(3)}-m]}g$ with $t=2\kappa$ into $e^{-\kappa(S-m^2)} = e^{-2\kappa H_A^{NR,1}}$ in the integrand of (4.22).

Then if we would use this further to represent $e^{-t[H^{(3)}-m]}g$ for $V\neq 0$, we might apply the Trotter–Kato product formula

$$e^{-t[H^{(3)}-m]} = \text{s-}\lim_{n\to\infty}\big(e^{-(t/n)[H_A^{(3)}-m]}e^{-(t/n)V}\big)^n, \tag{4.23}$$

for the sum $H^{(3)} - m = (H_A^{(3)} - m) + V$ to express the semigroup $e^{-t[H^{(3)}-m]}$ as a "limit", where convergence of the right-hand side usually takes place in strong operator topology as indicated. However it is not clear whether this procedure could further yield a path integral representation for $e^{-t[H^{(3)}-m]}g$.

In passing, let us insert a comment on the convergence of the Trotter–Kato product formula (4.23). It is now known that the convergence takes place even *in operator norm*, so long as the operator sum $(H_A^{(3)} - m) + V$ is selfadjoint on the common domain $D[H_A^{(3)}] \cap D[V]$ by the recent results in Ichinose–Tamura [IT1-01], Ichinose–Tamura–Tamura–Zagrebnov [ITTaZ-01] and also even pointwise convergence of the integral kernels in [IT2-04, 3-06] (cf. [I8-99]).

On the other hand, it does not seem possible to represent $e^{-t[H^{(3)]}-m]}g$ by path integral through directly applying Lévy process as we saw in the cases for $e^{-t[H^{(1)}-m])}g$ and $e^{-t[^{(2)}-m]}g$, because $H_A^{(3)}$ does not seem to be explicitly expressed by a pseudo-differential operator corresponding to a certain tractable symbol. It was in this situation that the problem of path integral representation for $e^{-t[H^{(3)]}-m]}g$ was studied first by DeAngelis–Serva [DeSe-90] and DeAngelis–Rinaldi–Serva [DeRSe-91] with use of *subordination /time-change* of Brownnian motion, and then by Nagasawa [N1-96, 2-97, 3-00]. Recently it has been more extensively studied by Hiroshima–Ichinose–Lőrinczi [HILo1-12, 2-12] (cf. [LoHB-11]) not only for the magnetic relativistic Schrödinger operator $H_A^{(3)}$ but also for Bernstein functions of the magnetic nonrelativistic Schrödinger operator and even with spin. In this connection, the problem on nonrelativistic limit was studied in [I1-87], [Sa1-90], [N1-97].

To proceed, let us explain about subordination (e.g., [Sa2, Chap.6, p. 197], [Ap-04/09, 1.3.2, p. 52]). Subordination is a transformation, through random time change, of a stochastic process to a new one which is a non-decreasing Lévy process independent of the original one, what is called *subordinator*. The new process is said to be *subordinate* to the original one.

As the original process, take $B^1(t)$, the one-dimensional standard Brownian motion, so that $B^1 \equiv B^1(\cdot)$ is a function belonging to the space $C_0([0,\infty)\to\mathbf{R})$ of real-valued continuous functions on $[0,\infty)$ satisfying $B^1(0) = 0$ and

$$e^{-t\frac{\xi^2}{2}} = \int_{C_0([0,\infty)\to\mathbf{R})} e^{i\xi B^1(t)} d\mu_0^S(B^1),$$

where μ_0^S is the Wiener measure on $C_0([0,\infty)\to\mathbf{R})$. Let $m \geq 0$ here, and for each B^1 and $t \geq 0$, put

$$T(t) \equiv T(t, B^1) := \inf\{\, s > 0\,;\, B^1(s) + ms = t\}. \tag{4.24}$$

Then $T \equiv T(\cdot)$ is a monotone, non-decreasing function on $[0,\infty)$ with $T(0) = 0$, belonging to $D_0([0,\infty)\to\mathbf{R})$ and so becoming a one-dimensional Lévy process, called *inverse Gaussian subordinator* for $m > 0$ and *Lévy subordinator* for $m = 0$. This correspondence defines a map $\hat{T}$ of $C_0([0,\infty)\to\mathbf{R})$ into $D_0([0,\infty)\to\mathbf{R})$ by $\hat{T}B^1(\cdot) = T(\cdot, B^1)$. Let ν_0 be the probability measure on $D_0([0,\infty)\to\mathbf{R})$ defined by $\nu_0(G) = \mu_0^S(\hat{T}^{-1}G)$ first for cylinder subsets $G \subset D_0([0,\infty)\to\mathbf{R})$ and then extended to more general subsets.

Proposition 4.4. (e.g., [Ap-04/09, Example 1.3.21, p. 54, and Exercise 2.2.10, p. 96; cf. Theorem 2.2.9, p. 95]) *The probability measure* ν_0 *satisfies*

$$e^{-t[\sqrt{2\sigma+m^2}-m]} = \int_{D_0([0,\infty)\to\mathbf{R})} e^{-T(t)\sigma} d\nu_0(T), \qquad \sigma \geq 0. \tag{4.25}$$

Proof. The proof will be not selfcontained, and need some basic facts about *martingale* and *stopping time* (e.g., [IkW2-81/89], [Sa2-99], [Ap-04/09], [DvC-00], [LoHB-11]). $T(t, B^1) = T(t)$ is a stopping time and then $B^1(T(t))$ is a *stopped random variable* belonging to $D_0([0,\infty)\to\mathbf{R})$. Then we see that, for $\theta \in \mathbf{R}$,

$$M_\theta(t) := e^{\theta B^1(t) - \frac{1}{2}\theta^2 t}$$

is a continuous martingale with respect to the natural filtration of Brownian motion $B^1(t)$. Further,

$$M_\theta((\hat{T}B^1)(t) \wedge n) = e^{B^1(T(t)\wedge n) - \frac{1}{2}\theta^2 T(t)\wedge n}$$

is also a martingale. Then by *Doob's optional stopping theorem* [Ap-04/09, Theorem 2.2.1, p. 92], for each $t > 0$, positive integer n and $\theta \geq 0$, we have

$$\begin{aligned}\int_{C_0([0,\infty)\to\mathbf{R})} M_\theta((\hat{T}B^1)(t) \wedge n) d\mu_0^S(B^1) &= \int_{C_0([0,\infty)\to\mathbf{R})} M_\theta((\hat{T}B^1)(0) \wedge n) d\mu_0^S(B^1) \\ &= \int_{C_0([0,\infty)\to\mathbf{R})} e^{\theta B^1(0)} d\mu_0^S(B^1) = 1.\end{aligned}$$

For each positive integer n and $t > 0$, put $\Omega_{n,t} := \{B^1 \in C_0([0,\infty) \to \mathbf{R})\,;\, T(t) = (\hat{T}B^1)(t) \leq n\}$. Then

$$\begin{aligned}&\int_{C_0([0,\infty)\to\mathbf{R})} M_\theta((\hat{T}B^1)(t) \wedge n) d\mu_0^S(B^1) \\ &= \int_{\Omega_{n,t}} M_\theta((\hat{T}B^1)(t) \wedge n) d\mu_0^S(B^1) + \int_{\Omega_{n,t}{}^c} M_\theta((\hat{T}B^1)(t) \wedge n) d\mu_0^S(B^1).\end{aligned}$$

Since, for $B^1(t)$, $(\hat{T}B^1)(t) = T(t) > n$ implies $B^1(t) < t - mn$, so that

$$\begin{aligned}\int_{(\Omega_{n,t})^c} M_\theta((\hat{T}B^1)(t) \wedge n) d\mu_0^S(B^1) &\leq e^{-\frac{1}{2}\theta^2 n} \int_{\Omega_{n,t}{}^c} e^{\theta B^1(n)} d\mu_0^S(B^1) \\ &\leq e^{-\frac{1}{2}\theta^2 n + \theta(t-mn)},\end{aligned}$$

which, for $\theta > 0$, tends to zero as $n \to \infty$. It follows by the monotone convergence theorem and (4.24) that

$$\begin{aligned} 1 &= \int_{C_0([0,\infty)\to\mathbf{R})} M_\theta((\hat{T}B^1)(t) \wedge n) d\mu_0^S(B^1) \\ &= \lim_{n\to\infty} \int_{\Omega_{n,t}} M_\theta((\hat{T}B^1)(t) \wedge n) d\mu_0^S(B^1) = \int_{C_0([0,\infty)\to\mathbf{R})} M_\theta((\hat{T}B^1)(t)) d\mu_0^S(B^1) \\ &= \int_{C_0([0,\infty)\to\mathbf{R})} e^{\theta\sqrt{m}[t-(\hat{T}B^1)(t)]-\frac{1}{2}\theta^2(\hat{T}B^1)(t)} d\mu_0^S(B^1), \end{aligned}$$

whence

$$\begin{aligned} e^{-\theta t} &= \int_{C_0([0,\infty)\to\mathbf{R})} e^{-\frac{1}{2}\theta(\theta+2m)(\hat{T}B^1)(t)} d\mu_0^S(B^1) \\ &= \int_{D_0([0,\infty)\to\mathbf{R})} e^{-\frac{1}{2}\theta(\theta+2m)T(t)} d\nu_0(T). \end{aligned}$$

Taking $\theta = \sqrt{2\sigma + m^2} - m$ yields the result, showing Proposition 4.4. □

This proposition implies that the characteristic function of the measure ν_0 is given by

$$e^{-tV(\rho)} = \int_{D_0([0,\infty)\to\mathbf{R})} e^{iT(t)\rho} d\nu_0(T), \qquad \rho \in \mathbf{R}\,, \tag{4.26}$$

$$\begin{aligned} V(\rho) &= \frac{\sqrt{m^4+4\rho^2}-m^2}{\sqrt{2}[(m^2+\sqrt{m^4+4\rho^2})^{1/2}+\sqrt{2}m]} - \frac{\sqrt{2}\rho}{(m^2+\sqrt{m^4+4\rho^2})^{1/2}}\, i \\ &= \frac{2\sqrt{2}\rho^2}{[(m^2+\sqrt{m^4+4\rho^2})^{1/2}+\sqrt{2}m](m^2+\sqrt{m^4+4\rho^2})} - \frac{\sqrt{2}\rho}{(m^2+\sqrt{m^4+4\rho^2})^{1/2}}\, i\,. \end{aligned}$$

To see this, first analytically extend $\sqrt{2\sigma+m^2}$ to the right-half complex plane $z := \sigma + i\rho,\ \sigma > 0,\ \rho \in \mathbf{R}$, and next we have $V(-\rho) = \lim_{\sigma\to+0} \sqrt{2(\sigma+i\rho)+m^2} - m$, of which the right-hand side is to be calculated. Then (4.26) follows with ρ replaced by $-\rho$. [cf. Using a subordinator $T(t)$ slightly different from (4.24), in [I9-12, (4.18), (4.19), (4.20), p.335] there are given a little different formulas corresponding to (4.25) and (4.26), $V(\rho)$. However, it contains an error; "ρ^2" in the expression for $V(\rho)$ there should be replaced by "$4\rho^2$".]

Now we are in a position to give a path integral representation for $e^{-t[H^{(3)}-m]}g$.

Theorem 4.5.

$$(e^{-t[H^{(3)}-m]}g)(x) = \int\int_{\substack{C_x([0,\infty)\to\mathbf{R}^d) \\ \times D_0([0,\infty)\to\mathbf{R})}} e^{-S^{(3)}(B,T;x,t)} g(B(T(t)))\, d\mu_x(B) d\nu_0(T), \tag{4.27}$$

$$
\begin{aligned}
S^{(3)}(B,T;x,t) &= i\int_0^{T(t)} A(B(s))\,dB(s) + \frac{i}{2}\int_0^{T(t)} \mathrm{div}A(B(s))ds \\
&\quad + \int_0^t V(B(T(s)))ds, \\
&\equiv i\int_0^{T(t)} A(B(s))\circ dB(s) + \int_0^t V(B(T(s)))ds,
\end{aligned} \tag{4.28}
$$

where μ_x is the Wiener measure on $C_x([0,\infty)\to\mathbf{R}^d)$ with characteristic function

$$
\exp\Big[-t\frac{|\xi|^2}{2}\Big] = \int_{C_x([0,\infty)\to\mathbf{R}^d)} e^{i(B(t)-x)\cdot\xi} d\mu_x(B). \tag{4.29}
$$

Remark. We note that for every pair $(B,T)\in C_x([0,\infty)\to\mathbf{R}^d)\times D_0([0,\infty)\to\mathbf{R})$ the path $B(T(s))$ in this theorem belongs to $D_x([0,\infty)\to\mathbf{R}^d)$, because it is right-continuous in $s\in[0,\infty)$ and has left-hand limit. The characteristic function of the product $\mu_x\times\nu_0$ of the probability measures is calculated with (4.29) as

$$
\begin{aligned}
&\int\int_{\substack{C_x([0,\infty)\to\mathbf{R}^d)\\ \times D_0([0,\infty)\to\mathbf{R})}} e^{i(B(T(t))-x)\cdot\xi}\, d\mu_x(B)d\nu_0(T) \\
&\quad = \int_{D_0([0,\infty)\to\mathbf{R})} \exp\Big[-T(t)\frac{|\xi|^2}{2}\Big]\, d\nu_0(T) = e^{-t[\sqrt{|\xi|^2+m^2}-m]},
\end{aligned} \tag{4.30}
$$

thus coinciding with (4.4), the characteristic function of the measure λ_x. This implies that these two processes on the two different probability spaces $\big(C_x([0,\infty)\to\mathbf{R}^d)\times D_0([0,\infty)\to\mathbf{R}),\ \mu_x\times\nu_0\big)$ and $\big(D_x([0,\infty)\to\mathbf{R}^d),\ \lambda_x\big)$ are identical in law, i.e., have the same finite-dimensional distributions, in fact, for $0<t_1<t_2<\cdots<t_n<\infty$ and $n=1,2,3,\ldots,$

$$
\begin{aligned}
&\int\int_{\substack{C_x([0,\infty)\to\mathbf{R}^d)\\ \times D_0([0,\infty)\to\mathbf{R})}} e^{i[(B(T(t_1))-x)\cdot\xi_1+(B(T(t_2))-x)\cdot\xi_2+\cdots+(B(T(t_n))-x)\cdot\xi_n]}\, d\mu_x(B)d\nu_0(T) \\
&= \int_{D_x([0,\infty)\to\mathbf{R}^d)} e^{i[(X(t_1)-x)\cdot\xi_1+(X(t_2)-x)\cdot\xi_2+\cdots+(X(t_n)-x)\cdot\xi_n]}\, d\lambda_x(X) \\
&= e^{-t_1[\sqrt{|\xi_1+\xi_2+\cdots+\xi_n|^2+m^2}-m]} e^{-(t_2-t_1)[\sqrt{|\xi_2+\cdots+\xi_n|^2+m^2}-m]}\cdot\cdots\cdot \\
&\qquad\qquad \times e^{-(t_n-t_{n-1})[\sqrt{|\xi_n|^2+m^2}-m]}.
\end{aligned}
$$

Therefore the former process may also be considered basically a Lévy process, but it is not clear whether one can rewrite the right-hand side of (4.27) as a process on the probability space $\big(D_x([0,\infty)\to\mathbf{R}^d),\ \lambda_x\big)$, replacing the function $S^{(3)}(B,T;x,t)$ of B, T, x, t in (4.28) with some function else of X, x, t appropriately written in terms of the Lévy space path X in $D_x([0,\infty)\to\mathbf{R}^d)$.

Proof of Theorem 4.5. We give only a sketch. The detail is referred to [IHLo1-12, Theorem 3.8, p. 1250013-14, with $\Psi(\sigma)=\sqrt{2\sigma+m^2}-m$]. We use Proposition 4.4 and the Feynman–Kac–Itô formula (4.2). Note that $H_A^{(3)} = \sqrt{2H_A^{NR}+m^2}$ with

$m > 0$. By the spectral theorem for the nonnegative selfadjoint operator H_A^{NR}, we have $H_A^{NR} = \int_{\mathrm{Spec}(H_A^{NR})} \sigma\, dE(\sigma)$, where $E(\cdot)$ is the spectral measure associated with H_A^{NR}. Then for $f, g \in L^2(\mathbf{R}^d)$

$$(f, e^{-t[H_A^{(3)}-m]}g) = \int_{\mathrm{Spec}(H_A^{NR})} e^{-t[\sqrt{2\sigma+m^2}-m]}\,(f, dE(\sigma)g).$$

Here we are using the *physicist's inner product* (f, g), which is anti-linear in f and linear in g. By Proposition 4.4 and again by the spectral theorem,

$$\begin{aligned}(f, e^{-t[H_A^{(3)}-m]}g) &= \int_{\mathrm{Spec}(H_A^{NR})} \int_{D_0([0,\infty)\to\mathbf{R})} e^{-T(t)\sigma} d\nu_0(T)\,(f, dE(\sigma)g)\\ &= \int_{D_0([0,\infty)\to\mathbf{R})} (f, e^{-T(t)H_A^{NR}} g)\, d\nu_0(T).\end{aligned}$$

Applying the Feynman–Kac–Itô formula (4.2) (for the case $V = 0$) to $e^{-T(t)H_A^{NR}}g$ in the third member, we have

$$\begin{aligned}&(f, e^{-t[H_A^{(3)}-m]}g)\\ &\quad= \int_{D_0([0,\infty)\to\mathbf{R})} d\nu_0(T) \int_{\mathbf{R}^d} dx\overline{f(B(0))} \int_{C_x([0,\infty)\to\mathbf{R}^d)}\\ &\qquad\qquad \times e^{-i\int_0^{T(t)} A(B(s))\circ dB(s)} g(B(T(t)))d\mu_x(B)\\ &\quad= \int_{\mathbf{R}^d} dx\overline{f(x)} \int\int_{\substack{C_x([0,\infty)\to\mathbf{R}^d)\\ \times D_0([0,\infty)\to\mathbf{R})}} e^{-i\int_0^{T(t)} A(B(s))\circ dB(s)} g(B(T(t)))\, d\mu_x(B) d\nu_0(T),\end{aligned}$$

where note $B(0) = x$. This proves the assertion when $V = 0$.

When $V \neq 0$, with partition of $[0, t]$: $0 = t_0 < t_1 < \cdots < t_n = t$, $t_j - t_{j-1} = t/n$, we can express $e^{-t[H^{(3)}-m]}g = e^{-t[(H_A^{(3)}-m)+V]}$ by the Trotter–Kato formula (4.23). Rewrite the product of these n operators by path integral with respect to the product of two probability measures $\nu_0(T) \cdot \mu_x(B)$ and note that $T(0) = T(t_0) = 0$, $B(0) = B(T(t_0)) = x$, then we have

$$\begin{aligned}&(f, \left(e^{-(t/n)[H_A^{(3)}-m]}e^{-(t/n)V}\right)^n g)\\ &\quad= \int_{\mathbf{R}^d} dx \int_{D_0([0,\infty)\to\mathbf{R})} d\nu_0(T) \int_{C_x([0,\infty)\to\mathbf{R}^d)} \overline{f(B(0))}\\ &\qquad\qquad \times e^{-i\sum_{j=1}^n \int_{T(t_{j-1})}^{T(t_j)} A(B(s))\circ dB(s)} e^{-\sum_{j=1}^n V(B(T(t_j)))\frac{t}{n}} g(B(t_n))\, d\mu_x(B).\end{aligned}$$

We see that, as $n \to \infty$, the left-hand side converges to $(f, e^{-t[H^{(3)}-m]}g)$, and the Lebesgue theorem shows the right-hand side converges as integral by the product measure $dx \times \nu_0(T) \times \mu_x(B)$, so that we obtain

$$(f, (e^{-t[H^{(3)}-m]}g) = \int_{\mathbf{R}^d} dx\overline{f(x)} \int\int_{\substack{C_x([0,\infty)\to\mathbf{R}^d) \\ \times D_0([0,\infty)\to\mathbf{R})}} e^{-S^{(3)}(B,T;x,t)} g(B(T(t)))\, d\mu_x(B)d\nu_0(T).$$

Hence or similarly we can also get (4.27)/(4.28) with f removed in the above inner products. □

4.2. Heuristic derivation of path integral formulas

After a brief introduction to *path integral*, we discuss, for the solution of the imaginary-time magnetic relativistic Schrödinger equation (4.3), how to heuristically derive its path integral formulas (4.9)/(4.10) in Theorem 4.1, (4.20)/(4.21) in Theorem 4.3 and (4.27)/(4.28) in Theorem 4.5.

4.2.1. What is *path integral*? It is a fabulous technique invented by Feynman in his Princeton 1942 thesis (see [Fey2-05]) and his 1948 paper [Fey1-48] to give alternative formulation of quantum mechanics. Its like has never been made before or since. In fact, though it is not mathematically rigorous, because of the universality of its idea, it has now come to prevail over all the domains in quantum physics. It is interesting to note, as he himself wrote in [48], that he came to the idea, "suggested by some of Dirac's remarks ([Di1-33, 2-35], [Di3-45]) concerning the relation of classical action to quantum mechanics." It is a special kind of *functional integral* like

$$\int e^{\frac{i}{\hbar}S(X)}\mathcal{D}[X] \tag{4.31}$$

on space of paths $X : [0,t] \ni s \mapsto X(s) \in \mathbf{R}^d$ with respect to a 'measure' $\mathcal{D}[X]$ on the space of these paths, where we are restoring the physical constant $\hbar = \frac{h}{2\pi}$ ($h > 0$: Planck's constant). $S(X)$ is time integral of the *Lagrangian* $L(X(s), \dot{X}(s))$ where $\dot{X}(s) = \frac{d}{ds}X(s)$:

$$S(X) = \int_0^t L(X(s), \dot{X}(s))ds,$$

which is an important quantity in classical mechanics, called *action* along the path X, having physical dimension of Planck's constant h so that $\frac{S(X)}{\hbar}$ becomes dimensionless.

We have in mind the nonrelativistic-quantum-mechanical motion of a particle in space $\mathbf{R}^d$ under influence of the scalar potential $V(x)$. In the previous sections, we let the particle have the special mass $m = 1$, but in this section, for a while, assume it to have general mass $m > 0$ so that we can see where m appears in the following description of its dynamics. Thus consider the Cauchy problem for the nonrelativistic Schrödinger equation for this particle with initial data $\psi(x, 0) = f(x)$:

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = \Big[-\frac{\hbar^2}{2m}\Delta + V(x)\Big]\psi(x,t), \quad t > 0, \quad x \in \mathbf{R}^d. \tag{4.32}$$

The solution is expressed as

$$\psi(x,t) = \int K(x,t;y,0)f(y)dy,$$

where $K(x,t;y,0)$ is integral kernel, called *fundamental solution* or *propagator*.

Feynman writes down this important quantity $K(x,t;s,y)$ as an 'integral'

$$K(x,t;y,0) = \int_{\{X:\,X(0)=y,X(t)=x\}} e^{\frac{i}{\hbar}S(X)}\mathcal{D}[X], \tag{4.33}$$

where in the present case $L(X(s),\dot{X}(s)) = \frac{m}{2}\dot{X}(s)^2 - V(X(s))$, so that $S(X)$ is given by

$$S(X) = \int_0^t \Big[\frac{m}{2}\dot{X}(s)^2 - V(X(s))\Big]ds. \tag{4.34}$$

$\mathcal{D}[X]$ stands for a uniform 'measure', if it exists, on the space of paths $X(\cdot)$ starting from position y in space at time 0 to arrive at position x in space at time t, *formally* to be given by the infinite product of continuously-many number of the Lebesgue measures $dX(\tau)$ on space $\mathbf{R}^d$ for each individual τ:

$$\mathcal{D}[X] := \text{“constant”} \times \prod_{0<\tau<t} dX(\tau).$$

Here the "constant" should be something like $\big(\frac{im}{2\pi\hbar(\delta t)}\big)^{\frac{d}{2}\cdot(\frac{t}{\delta t}-1)}$ with δt being some infinitesimal quantity of time, if one dares to try to write it, wondering what it means at all, but one may infer something from around (4.37) below. The right-hand side of (4.33) is what is called *Feynman path integral* or, nowadays simply, *path integral*.

To explain this, Feynman put the following *Two Postulates* which turn out to be equivalent to get the above expression (4.33) for $K(x,t;y,0)$, so that, for $f,\, g \in L^2(\mathbf{R}^d)$,

$$(f, \psi(\cdot,t)) = (f, e^{-\frac{it}{\hbar}[-\frac{\hbar^2}{2m}\Delta+V]}g) = \int\int \overline{f(x)}K(x,t;y,0)g(y)dxdy.$$

Feynman's Two Postulates

(i) $K(x,t;y,0)$ is the *total probability amplitude* for the event that the particle starts from position y at time 0 and arrives at position x at time t. If $\varphi[X]$ stands for the *probability amplitude* for the event that it does this motion *along each individual path* $X(\cdot)$, $K(x,t;y,0)$ is the sum of the $\varphi[X]$ over all these paths $X(\cdot)$:

$$K(x,t;y,0) = \sum_{\{X:\,X(0)=y,X(t)=x\}} \varphi[X]. \tag{4.35}$$

(ii) The contribution $\varphi[X]$ from each $X(\cdot)$ to the total probability amplitude $K(x,t;y,0)$ is given by

$$\varphi[X] = Ce^{\frac{i}{\hbar}S(X)}, \tag{4.36}$$

where C is a constant independent of path X.

These two postulates can be paraphrased: In quantum mechanics there rules the Principle of Democracy that each individual path $X(\cdot)$ contributes to the total probability amplitude $K(x,t;y,0)$ with *equal weight* (*absolute value* in mathematics) and its personality is expressed by its *phase* (*argument* in mathematics).

In this respect, in classical mechanics there does not rule Principle of Democracy, because the particle takes a *particular path* between two space-time points $(y,0)$ and (x,t) which makes the action $S(X)$ stationary, called *classical trajectory.* It is the path determined by Euler–Lagrange equation or, in the present case, Newton's equation of motion: $m\frac{d^2}{ds^2}X(s) = -\nabla V(X(s))$.

The most important characteristic feature of these postulates lies in equation (4.36), which says that the amplitude $\varphi[X]$ is proportional to the phase $e^{\frac{i}{\hbar}S(X)}$. The phrase "proportional to" is that which Feynman determined to substitute for what Dirac had meant by the phrase "analogous to" in [Di1-33, 2-35], [Di3-45] far before Feynman, by showing after his own analysis and deliberation that *indeed this exponential function could be used in this manner directly* (see Preface of [FeyHi-65]).

In classical mechanical circumstances, $\hbar$ is so small compared with other physical quantities that one may ignore and think of it as zero. The amazing thing is that this 'integral' (4.33) can let us see how the transition is going to classical mechanics as $\hbar$ tends to zero. Namely, when $\hbar$ tends to zero, if the stationary phase method should be valid for this 'integral' (4.33), then the 'integral' would turn out to receive the most crucial contribution from the path which makes the action $S(X)$ stationary, i.e., the classical trajectory (mentioned above) and its neighboring paths.

4.2.2. How to make it mathematics? Here we refer, among others, only to two methods; one is by finite-dimensional approximation, and the other by imaginary-time path integral. In fact, it is by the first method that Feynman himself confirmed his idea of path integral. He calculated $K(x,t;y,0)$ by time-sliced approximation, making partition of the time interval $[0,t]$: $0 = t_0 < t_1 < \cdots < t_n = t$, $(t_j - t_{j-1} = t/n)$, $x_j := X(t_j)$, $x_0 = X(0) = y$, $x_n = X(t) = x$, as the limit of

$$K_n(x,t;y,0) := \frac{\int_{(\mathbf{R}^\mathbf{d})^{n-1}} \exp\{\frac{it}{\hbar n}\sum_{j=0}^{n-1}[\frac{m}{2}(\frac{x_{j+1}-x_j}{t/n})^2 - V(x_j)]\}dx_1\cdot\cdots\cdot dx_{n-1}}{\int_{(\mathbf{R}^\mathbf{d})^n} \exp\{\frac{it}{\hbar n}\sum_{j=0}^{n-1}\frac{m}{2}(\frac{x_{j+1}-x_j}{t/n})^2\}dx_1\cdot\cdots\cdot dx_{n-1}dx_n} \tag{4.37}$$

as $n \to \infty$, to ascertain it to satisfy the Schrödinger equation (4.32). Note that the denominator of the right-hand side of (4.37) is equal to $\left(\frac{2\pi i\hbar\frac{t}{n}}{m}\right)^{\frac{d}{2}\cdot n}$.

The second method is the one which the present article is mainly concerning. We note with (4.33) that the solution $\psi(x,t)$ of the Schrödinger equation (4.32) turns out to be given by a heuristic path integral

$$\psi(x,t) = \int_{\mathbf{R}^d} K(x,t;y,0)f(y)dy = \int_{\{X:\, X(t)=x\}} e^{\frac{i}{\hbar}S(X)} f(X(0))\mathcal{D}[X]. \tag{4.38}$$

However, one should know that the 'measure' $\mathcal{D}[X]$ itself in general does not exist in this situation as a countably additive measure. Therefore we cannot go further. But if we rotate everything by $-90^\circ : t \to -it$ (real-time t to imaginary-time $-it$) in complex t-plane (see Figure 1), i.e., if we go from our *Minkowski* space-time to *Euclidian* space-time, the situation will change. Before actually doing it, for simplify put $\hbar = 1$. Then, as our rotation also converts ds to $-ids$, so does it $\dot{X}(s) = \frac{dX(s)}{ds}$ to $i\dot{X}(s) = \frac{dX(s)}{-ids}$ [where we don't mind thinking of "$X(-is)$" as $X(s)$ again], so that $iS(X)$, the action $S(X)$ in (4.3) multiplied by $i = \sqrt{-1}$, is converted to time integral of the *Hamiltonian*: $-\int_0^t [\frac{m}{2}\dot{X}(s)^2 + V(X(s))]ds$. Simultaneously, our (real-time) Schrödinger equation (4.32) is converted to the imaginary-time Schrödinger equation, i.e., heat equation [where writing $u(x,t)$ for $\psi(x,-it)$]:

$$\frac{\partial}{\partial t}u(x,t) = \left[\frac{1}{2m}\Delta - V(x)\right]u(x,t), \quad t > 0, \quad x \in \mathbf{R}^d. \tag{4.39}$$

Now we are going to get to the so-called *Feynman–Kac formula*. To this end, we replace the paths used so far by the time-reversed paths $X_0(s) := X(t-s),\ 0 \le s \le t$, so that $X_0(0) = X(t) = x,\ X_0(y) = X(0) = y$. Then $K(x,t;y,0)$ is changed to

$$K^E(x,t;y,0) := \int_{\{X_0:\, X_0(0)=x, X_0(t)=y\}} e^{-\int_0^t [\frac{m}{2}\dot{X}_0(s)^2 + V(X_0(s))]ds} \mathcal{D}[X_0]. \tag{4.40}$$

where the superscript "E" is attributed to "Euclidian", and $K^E(x,t;y,0)$ should become the integral kernel for the heat equation (4.39). In passing we quickly insert here: if one were to follow the first method by Feynman as (4.37), one could also define $K^E(x,t;y,0)$ as the limit as $n \to \infty$ of

$$K_n^E(x,t;y,0) := \frac{\int_{(\mathbf{R}^\mathbf{d})^{n-1}} \exp\{-\frac{t}{n}\sum_{j=0}^{n-1}[\frac{m}{2}(\frac{x_{j+1}-x_j}{t/n})^2 + V(x_j)]\}dx_1 \cdot \cdots \cdot dx_{n-1}}{\int_{(\mathbf{R}^\mathbf{d})^n} \exp\{-\frac{t}{n}\sum_{j=0}^{n-1} \frac{m}{2}(\frac{x_{j+1}-x_j}{t/n})^2\}dx_1 \cdot \cdots \cdot dx_{n-1}dx_n}, \tag{4.41}$$

where $t_j - t_{j-1} = t/n\,(j = 1,2,\ldots,n)$; $x_j = X_0(t_j)$, $x_0 = X_0(0) = x$, $x_n = X_0(t) = y$.

We infer from (4.40) that the solution of the Cauchy problem for (4.39) with initial data $u(x,0) = g(x)$ should be given by the following path integral

$$\begin{aligned} u(x,t) &= \int_{\mathbf{R}^d} K^E(x,t;y,0)g(y)dy \\ &= \int_{\{X_0:\, X_0(0)=x\}} e^{-\int_0^t [\frac{m}{2}\dot{X}_0(s)^2 + V(X_0(s))]ds} g(X_0(t))\mathcal{D}[X_0]. \end{aligned} \tag{4.42}$$

Here we have tacitly identified the two 'integrals':

$$\int_{\mathbf{R}^d} dy \int_{\{X_0 \colon X_0(0)=x, X_0(t)=y\}} \cdots \mathcal{D}[X_0] \quad \sim \quad \int_{\{X_0 \colon X_0(0)=x\}} \cdots \mathcal{D}[X_0].$$

Needless to say, when the scalar potential $V(x)$ is absent, $K^E(x,t;y,0)$ becomes the heat kernel $\left(\frac{2\pi t}{m}\right)^{-d/2} e^{-\frac{m}{2t}|x-y|^2}$, which is obtained as the inverse Fourier transform of the left-hand side of (4.29), or by calculating the integrals (4.41) and taking the limit $n \to \infty$. Note that the denominator of (4.41) is equal to $\left(\frac{2\pi \frac{t}{n}}{m}\right)^{\frac{d}{2}\cdot n}$. By (4.40) we also see it have the following heuristic expression on the right-hand side

$$\frac{e^{-\frac{m}{2t}|x-y|^2}}{\left(\frac{2\pi t}{m}\right)^{d/2}} = \int_{\{X_0 \colon X_0(0)=x, X_0(t)=y\}} e^{-\int_0^t \frac{m}{2}\dot{X}_0(s)^2 ds} \mathcal{D}[X_0].$$

Remarkable is that Wiener, already around 1923, had constructed, for each individual $x \in \mathbf{R}^d$, a countably additive measure μ_x with $m = 1$ (but of course valid for every $m > 0$) on the space $C_x := C_x([0,\infty) \to \mathbf{R}^d)$ of the continuous paths (*Brownian motions*) $B : [0,\infty) \ni s \mapsto B(s) \in \mathbf{R}^d$ starting from $B(0)=x$ at time $t = 0$. Further μ_x is a probability measure on C_x with characteristic function (4.29), and now is called *Wiener measure*.

Around 1947, Kac, who had been at Cornell University as Feynman and heard his lecture at the Physics Colloquium, struck upon the very idea of using the Wiener measure to represent the solution $u(x,t)$ of the Cauchy problem for the heat equation (4.39) (with $m = 1$) with initial data $u(x,0) = g(x)$ as a first mathematical rigorous, *genuine functional integral*

$$u(x,t) = \int K^E(x,t;y,0) g(y) dy = \int_{C_x([0,\infty)\to\mathbf{R}^d)} e^{-\int_0^t V(B(s))ds} g(B(t)) d\mu_x(B), \tag{4.43}$$

the same formula as (4.1) already mentioned at the top of this section. This is the *Feynman–Kac formula* [Kac-66/80] mentioned in advance. Thus, identify the path $X_0(\cdot)$ appearing on the right-hand side of (4.40)/(4.42) with the continuous path $B(\cdot)$ in the space $C_x([0,\infty)\to\mathbf{R}^d)$, then the Wiener measure μ_x turns out to be constructed from the factor "$e^{-\int_0^t \frac{m}{2}\dot{B}(s)^2 ds}\mathcal{D}[B]$" (with $m = 1$) on the right-hand side of (4.40)/(4.42).

4.2.3. The case for relativistic Schrödinger equation. We begin with the relativistic Schrödinger equation for a relativistic particle of mass m with positive energy in an electromagnetic field:

$$i\hbar\frac{\partial}{\partial t}\psi(x,t) = [H - m]\psi(x,t), \quad t > 0, \quad x \in \mathbf{R}^d, \tag{4.44}$$

where H is one of the relativistic Schrödinger operators $H^{(1)}$, $H^{(2)}$ and $H^{(3)}$ corresponding to the classical symbol $\sqrt{(\xi - A(x))^2 + m^2} + V(x)$. This equation (4.44) was already briefly mentioned at the top of Section 4.1. However, here for the moment we go with the quantization "$\xi \to -i\hbar\nabla$" with $\hbar$ recovered, but not

"$\xi \to -i\nabla$" used there. In this case it is more appropriate to use the method of *phase space path integral* or *Hamiltonian path integral* (Feynman [Fey-65, p. 125], Garrod [G-66], Mizrahi [M-78]):

$$\int e^{\frac{i}{\hbar}S(\Xi,X)}\mathcal{D}[\Xi]\mathcal{D}[X] \tag{4.45}$$

with a 'measure' $\mathcal{D}[\Xi]\mathcal{D}[X]$ on the space of phase space paths (Ξ, X), pairs of momentum path $\Xi(s)$ and position path $X(s)$ on the phase space $\mathbf{R}^d \times \mathbf{R}^d$, and with *action* written with each pair $(\Xi(s), X(s))$. Then, under this circumstance, the previous path integral (4.31), (4.33) in the nonrelativistic case is also called *configuration path integral*.

The solution $\psi(x,t)$ of the Cauchy problem for (4.44) with initial data $\psi(x,0) = f(x)$ can be written as $\psi(x,t) = \int K(x,t;y,0)f(y)dy$ with integral kernel $K(x,t;y,0)$ called *fundamental solution or propagator*. Then the method of phase space path integral or Hamiltonian path integral assumes $K(x,t;y,0)$ to have the following path integral representation:

$$K(x,t;y,0) = \int_{\{(\Xi,X);\, X(0)=y, X(t)=x,\, \Xi:\,\text{arbitrary}\}} e^{\frac{i}{\hbar}S(\Xi(s),X(s))}\mathcal{D}[\Xi]\mathcal{D}[X]\,. \tag{4.46}$$

Here the *action* $S(\Xi, X)$ along the phase space path (Ξ, X) is given by

$$S(\Xi,X) = \int_0^t \Big[\Xi(s)\cdot\dot{X}(s) - \Big(\sqrt{(\Xi(s)-A(X(s)))^2+m^2} - m + V(X(s))\Big)\Big]ds, \tag{4.47}$$

where $\dot{X}(s) = \frac{d}{ds}X(s)$ in the same way as in the nonrelativistic case (4.34). $\mathcal{D}[\Xi]\mathcal{D}[X]$ is a uniform 'measure', if it exists, on the space of phase space paths $(\Xi, X) : [0,t] \ni s \mapsto (\Xi(s), X(s)) \in \mathbf{R}^d \times \mathbf{R}^d$ with $X(0) = y, X(t) = x$, but Ξ being unrestricted and so arbitrary, *formally* to be given by the infinite product of continuously-many number of the Lebesgue measures $d\Xi(\tau)dX(\tau)$ (precisely, divided by $(2\pi)^d$) on phase space $\mathbf{R}^{2d} = \mathbf{R}^d \times \mathbf{R}^d$ for each individual τ:

$$\mathcal{D}[\Xi]\mathcal{D}[X] := \prod_{0<\tau<t}\frac{d\Xi(\tau)dX(\tau)}{(2\pi)^d}.$$

In this 'integral' (4.46) we make the transform of variables (paths): $\Xi'(s) = \Xi(s) - A(X(s))$ and $X'(s) = X(s)$, where we note the *formal* Jacobi determinant $\frac{\partial(\Xi(s)\,,\,X(s))}{\partial(\Xi'(s),X'(s))}$ of this transform is 1. Write $\Xi(s)$ for $\Xi'(s)$ and $X(s)$ for $X'(s)$ again, then (4.46) becomes

$$K(x,t;y,0) = \int_{\{(\Xi,X);\, X(0)=y, X(t)=x,\, \Xi:\,\text{arbitrary}\}} \tag{4.48}$$
$$\times\, e^{\frac{i}{\hbar}\int_0^t \left[(\Xi(s)+A(X(s))\cdot\dot{X}(s) - \left(\sqrt{\Xi(s)^2+m^2}-m+V(X(s))\right)\right]ds}\mathcal{D}[\Xi]\mathcal{D}[X].$$

We want to find a path integral formula for the solution of the imaginary-time magnetic relativistic Schrödinger equation (4.3). For simplicity we put $\hbar = 1$ as before. We go from real time t to imaginary time $-it$. This procedure also converts

ds to $-ids$ and so $\dot{X}(s) = \frac{d}{ds}X(s)$ to $i\dot{X}(s) = \frac{dX(s)}{-ids}$ [where we don't mind thinking of "$\Xi(-is),\ X(-is)$" as $\Xi(s),\ X(s)$, respectively, again]. Then we replace the phase space paths used so far by the time-reversed phase space paths: $X_0(s) := X(t-s),\ \Xi_0(s) := \Xi(t-s),\ 0 \le s \le t$, so that $X_0(0) = X(t) = x,\ X_0(y) = X(0) = y$. As a result, (4.46) is changed to

$$K^E(x,t;y,0) := \int_{\{(\Xi_0,X_0);\, X_0(0)=x, X_0(t)=y,\, \Xi\colon \text{arbitrary}\}} \times e^{\int_0^t \left[i(\Xi_0(s)+A(X_0(s))\cdot\dot{X}_0(s) - \left(\sqrt{\Xi_0(s)^2+m^2}-m+V(X_0(s))\right)\right]ds} \mathcal{D}[\Xi_0]\mathcal{D}[X_0]. \tag{4.49}$$

At this final stage we rewrite $\Xi_0(s),\ X_0(s)$ as $\Xi(s),\ X(s)$ again. Thus we have heuristically arrived, for the solution $u(x,t)$ of the Cauchy problem for (4.3) with initial data $u(x,0) = g(x)$, at the following path integral representation:

$$\begin{aligned} u(x,t) &= (e^{-t[H-m]}g)(x) = \int K^E(x,t;y,0)g(y)dy \\ &= \int_{\{X(0)=x\}} e^{\int_0^t \left[i(\Xi(s)+A(X(s)))\cdot\dot{X}(s) - \left(\sqrt{\Xi(s)^2+m^2}-m+V(X(s))\right)\right]ds} \\ &\qquad \times g(X(t))\mathcal{D}[\Xi]\mathcal{D}[X] \\ &= \int_{\{X(0)=x\}} e^{\int_0^t \left[iA(X(s))\cdot\dot{X}(s) - V(X(s))\right]ds} \\ &\qquad \times e^{\int_0^t \left[i\Xi(s)\cdot\dot{X}(s) - \left(\sqrt{\Xi(s)^2+m^2}-m\right)\right]ds} g(X(t))\mathcal{D}[\Xi]\mathcal{D}[X]. \end{aligned} \tag{4.50}$$

Now we ask whether our path integral formulas, (4.9)/(4.10) in Theorem 4.1, (4.20)/(4.21) in Theorem 4.3 and (4.27)/(4.28) in Theorem 4.5, can be well derived or at least well inferred from this formal expression of 'integral' (4.50). First of all, if both the vector and scalar potentials $A(x)$ and $V(x)$ are absent, (4.50) is reduced to

$$\begin{aligned} u(x,t) &= (e^{-t[\sqrt{-\Delta+m^2}-m]}g)(x) = \int k_0(x-y,t)g(y)dy \\ &= \int_{\{X(0)=x\}} e^{\int_0^t \left[i\Xi(s)\cdot\dot{X}(s) - \left(\sqrt{\Xi(s)^2+m^2}-m\right)\right]ds} g(X(t))\mathcal{D}[\Xi]\mathcal{D}[X], \end{aligned} \tag{4.51}$$

where $k_0(x-y,t)$ is the integral kernel of the semigroup $e^{-t[\sqrt{-\Delta+m^2}-m]}$ in (3.3), and, similarly to the nonrelativistic case, we have identified the two 'integrals':

$$\begin{aligned} &\int_{\mathbf{R}^d} dy \int_{\{(\Xi,X);\, X(0)=x, X(t)=y,\, \Xi\colon \text{arbitrary}\}} \cdots \mathcal{D}[\Xi]\mathcal{D}[X] \\ &\quad \sim \int_{\{(\Xi,X);\, X(0)=x,\, \Xi\colon \text{arbitrary}\}} \cdots \mathcal{D}[\Xi]\mathcal{D}[X]. \end{aligned}$$

Noting that the second and/or third member of (4.50) is equal to

$$\int_{D_x([0,\infty)\to\mathbf{R}^d)} g(X(t))d\lambda_x(X),$$

we see that the factor

$$\exp\Big\{\int_0^t \Big[i\Xi(s)\cdot\dot{X}(s) - \Big(\sqrt{\Xi(s)^2+m^2}-m\Big)\Big]ds\Big\}\mathcal{D}[\Xi]\mathcal{D}[X] \tag{4.52}$$

turns out to be identified with the probability measure λ_x, (4.4) introduced in Section 4.1, connected with the Lévy process concerned. Next, we shall see that, since there is no problem for the factor $e^{-\int_0^t V(X(s))ds}$, the problem lies only in how to interpret and understand the factor

$$e^{i\int_0^t A(X(s))\cdot\dot{X}(s)ds} = \prod_{j=1}^n e^{i\int_{t_{j-1}}^{t_j} A(X(s))\cdot\dot{X}(s)ds},$$

when dividing the time interval $[0,t]$ into n equal small subintervals $[t_0,t_1]$, ..., $[t_{n-1},t_n]$ with $t_j = jt/n$, $j = 0,1,2,\dots,n$, in fact, whether, for small interval $[t_{j-1},t_j]$ or large n, the factor $e^{i\int_{t_{j-1}}^{t_j} A(X(s))\cdot\dot{X}(s)ds}$ can allow a good approximation to be suggested by the obtained path integral formulas for $H^{(1)}$, $H^{(2)}$ and $H^{(3)}$.

(1) First we consider the case for $H^{(1)}$ by approximating the factor

$$\exp\Big[i\int_{t_{j-1}}^{t_j} A(X(s))\cdot\dot{X}(s)ds\Big] \text{ by } \exp\Big[iA\Big(\frac{X(t_{j-1})+X(t_j)}{2}\Big)\cdot(X(t_j)-X(t_{j-1}))\Big]$$

on each subinterval $[t_{j-1},t_j]$ ("midpoint prescription"). Then the last member of (4.15) is expected to be the limit $n\to\infty$ of

$$\overbrace{\int_{\mathbf{R}^{2d}}\cdots\int_{\mathbf{R}^{2d}}}^{n\text{ times}}\Big(e^{i\sum_{j=1}^n(\Xi(t_j)+A(\frac{X(t_{j-1})+X(t_j)}{2})\cdot(X(t_j)-X(t_{j-1}))}$$
$$\times e^{-\sum_{j=1}^n[\sqrt{\xi_j^2+m^2}-m+V(\frac{X(t_{j-1})+X(t_j)}{2})]\frac{t}{n}}\Big)g(X(t_n))\prod_{j=1}^n\frac{d\Xi(t_j)dX(t_j)}{(2\pi)^d}$$

$$=\overbrace{\int_{\mathbf{R}^{2d}}\cdots\int_{\mathbf{R}^{2d}}}^{n\text{ times}}\Big(e^{i\sum_{j=1}^n[(\Xi(t_j)\cdot(X(t_j)-X(t_{j-1}))-(\sqrt{\xi_j^2+m^2}-m)\frac{t}{n}]}$$
$$\times e^{i\sum_{l=1}^n[A(\frac{X(t_{l-1})+X(t_l)}{2})\cdot(X(t_j)-X(t_{j-1}))-V(\frac{X(t_{l-1})+X(t_l)}{2})\frac{t}{n}]}\Big)$$
$$\times g(X(t_n))\prod_{j=1}^n\frac{d\Xi(t_{j-1})dX(t_{j-1})}{(2\pi)^d},\qquad X(0)=X(t_0)=x. \tag{4.53}$$

Then putting $\xi_j = \Xi(t_j),\ x_j = X(t_j)$ makes (4.50) equal to

$$\overbrace{\int_{\mathbf{R}^{2d}} \cdots \int_{\mathbf{R}^{2d}}}^{n \text{ times}} \prod_{j=1}^{n} e^{i(x_j - x_{j-1})\cdot\xi_j} e^{-[\sqrt{\xi_j^2+m^2}-m]\frac{t}{k}}$$
$$\times \exp\Big\{ i \sum_{l=1}^{n} \Big[A\Big(\frac{x_{l-1}+x_l}{2}\Big) \cdot (x_l - x_{l-1}) - V\Big(\frac{x_{l-1}+x_l}{2}\Big)\frac{t}{n}\Big)\Big]\Big\}$$
$$\times\, g(x_n) \prod_{j=1}^{n} \frac{d\xi_j dx_j}{(2\pi)^d}, \qquad x_0 = x. \tag{4.54}$$

Performing all the $d\xi_j$ integrals yields

$$\overbrace{\int_{\mathbf{R}^{d}} \cdots \int_{\mathbf{R}^{d}}}^{n \text{ times}} k_0(x_0 - x_1, t/n) k_0(x_1 - x_2, t/n) \cdot \cdots \cdot k_0(x_{n-1} - x_n, t/n)$$
$$\times \exp\Big\{ - \sum_{l=1}^{n} \Big[iA\Big(\frac{x_{l-1}+x_l}{2}\Big) \cdot (x_{l-1} - x_l) + V\Big(\frac{x_{l-1}+x_l}{2}\Big)\frac{t}{n}\Big)\Big]$$
$$\times\, g(x_n) dx_1 \cdot \cdots \cdot dx_n, \qquad x_0 = x, \tag{4.55}$$

where $k_0(x,t)$ is the integral kernel of $e^{-t[\sqrt{-\Delta+m^2}-m]}$ in (3.3). Note that (4.55) is the same as the second member of (4.15), which was shown in Proposition 4.2 to converge to $e^{-t[H^{(1)}-m]}g$. Therefore we may think that the expression (4.9) with (4.10) is heuristically connected with (4.50) in the limit $n \to \infty$ of the expression (4.55) which should be the path integral formula for $e^{-t[H^{(1)}-m]}g$ in Theorem 4.1.
(2) Next we consider the case for $H^{(2)}$ by approximating the factor

$$\exp\Big[i \int_{t_{j-1}}^{t_j} A(X(s)) \cdot \dot{X}(s) ds \Big]$$

by

$$\exp\Big[i \int_0^1 A\big((1-\theta)X(t_j) + \theta X(t_{j-1})\big) \cdot (X(t_j) - X(t_{j-1})) d\theta \Big]$$

on each subinterval $[t_{j-1}, t_j]$. The same arguments as in (1) above will show the expression (4.20) with (4.21) is also heuristically connected with (4.50), leading to the path integral formula (4.20) with (4.21) for $e^{-t[H^{(2)}-m]}g$ in Theorem 4.3.

(3) Finally, we come to the case for $H^{(3)}$. Indeed, (4.27)/(4.28) is a mathematically rigorous, beautiful path integral but it does not seem to be one which can be heuristically deduced from the formal expression of 'integral' (4.50). We could not think the factor $\exp\Big[i \int_{t_{j-1}}^{t_j} A(X(s)) \cdot \dot{X}(s) ds \Big]$ can allow a good approximation to be suggested by (4.27)/(4.28) for $H^{(3)}$. It is because $H_A^{(3)}$ does not seem to be so explicitly well expressed by a pseudo-differential operator defined through a certain *tractable symbol* as $H_A^{(1)}$ and $H_A^{(2)}$.

5. Summary

Finally, we will collect here, as summary, the three path integral representation formulas in Theorems 4.1, 4.3, 4.5 so as to be able to explicitly see how they are x-dependent. To do so, we replace the x-dependent path space $D_x \equiv D_x([0,\infty) \to \mathbf{R}^d)$ / $C_x \equiv C_x([0,\infty) \to \mathbf{R}^d)$ (with probability measure λ_x / μ_x) *by* the x-independent path space $D_0 \equiv D_0([0,\infty) \to \mathbf{R}^d)$ / $C_0 \equiv C_0([0,\infty) \to \mathbf{R}^d)$ of the paths $X(s)$ / $B(s)$ starting from 0 in space $\mathbf{R}^d$ at time $s = 0$ (with probability measure λ_0 / μ_0), respectively. Namely, in the path integral representation formulas in these three theorems, we make change of space, probability measure and paths by translation x:

$$D_x \to D_0,\ \lambda_x \to \lambda_0,\ X(s) \to X(s) + x,$$

$$C_x \to C_0,\ \mu_x \to \mu_0,\ B(s) \to B(s) + x,\ B(T(s)) \to B(T(s)) + x,$$

$$(4.9) : (e^{-t[H^{(1)}-m]}g)(x) = \int_{D_0([0,\infty)\to\mathbf{R}^d)} e^{-S^{(1)}(X;x,t)} g(X(t) + x)\, d\lambda_0(X),$$

$$\begin{aligned} S^{(1)}(X;x,t) = {} & i\int_0^{t+}\int_{|y|>0} A\left(X(s-) + x + \frac{y}{2}\right) \cdot y\, \widetilde{N}_X(dsdy) \\ & + i\int_0^t\int_{|y|>0} \left[A\left(X(s) + x + \frac{y}{2}\right) - A(X(s) + x)\right] \cdot y\, dsn(dy) \\ & + \int_0^t V(X(s) + x)ds\,; \end{aligned}$$

$$(4.20) : (e^{-t[H^{(2)}-m]}g)(x) = \int_{D_0([0,\infty)\to\mathbf{R}^d)} e^{-S^{(2)}(X;x,t)} g(X(t) + x)\, d\lambda_0(X),$$

$$\begin{aligned} S^{(2)}(X;x,t) = {} & i\int_0^{t+}\int_{|y|>0} \left(\int_0^1 A(X(s-) + x + \theta y)d\theta\right) \cdot y\, \widetilde{N}_X(dsdy) \\ & + i\int_0^t\int_{|y|>0} \left[\int_0^1 A(X(s) + x + \theta y)d\theta - A(X(s)\right] \cdot y\, dsn(dy) \\ & + \int_0^t V(X(s) + x)ds\,; \end{aligned}$$

$$\begin{aligned} (4.27) : (e^{-t[H^{(3)]}-m]}g)(x) = {} & \int\int_{\substack{C_0([0,\infty)\to\mathbf{R}^d) \\ \times D_0([0,\infty)\to\mathbf{R})}} \\ & \times e^{-S^{(3)}(B,T;x,t)} g(B(T(t))+x)\, d\mu_0(B) d\nu_0(T), \end{aligned}$$

$$\begin{aligned} S^{(3)}(B,T;x,t) = {} & i\int_0^{T(t)} A(B(s) + x) \cdot dB(s) + \frac{i}{2}\int_0^{T(t)} \mathrm{div}A(B(s)+x)ds \\ & + \int_0^t V(B(T(s))+x)ds, \\ \equiv {} & i\int_0^{T(t)} A(B(s) + x) \circ dB(s) + \int_0^t V(B(T(s)) + x)ds. \end{aligned}$$

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Some Aspects of Large Time Behavior of the Heat Kernel: An Overview with Perspectives

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Dedicated to Professor Michael Demuth on the occasion of his 65th birthday

Abstract. We discuss a variety of developments in the study of large time behavior of the positive minimal heat kernel of a time-independent (not necessarily symmetric) second-order parabolic operator defined on a domain $M \subset \mathbb{R}^d$, or more generally, on a noncompact Riemannian manifold M. Our attention is mainly focused on *general* results in general settings.

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Keywords. Heat kernel, Green function, parabolic Martin boundary, positive solutions, ratio limit.

Contents

1. Introduction

The large time behavior of the heat kernel of a second-order parabolic operator has been extensively studied over the recent decades (see for example the following monographs and survey articles [6, 11, 17, 18, 20, 25, 29, 37, 54, 55, 57, 59, 62, 63, 64], and references therein). The purpose of the present paper is to review a variety of developments in this area, and to point out a number of their consequences. Our attention is mainly focused on *general* results in general settings. Still, the selection of topics in this survey is incomplete, and is according to the author's working experience and taste. The reference list is far from being complete and serves only this exposé.

Let P be a general linear, second-order, elliptic operator defined on a domain $M \subset \mathbb{R}^d$ or, more generally, on a noncompact, connected, Riemannian manifold M of dimension $d \geq 1$. Denote the cone of all positive solutions of the equation $Pu = 0$ in M by $\mathcal{C}_P(M)$. The *generalized principal eigenvalue* is defined by

$$\lambda_0 = \lambda_0(P, M) := \sup\{\lambda \in \mathbb{R} \mid \mathcal{C}_{P-\lambda}(M) \neq \emptyset\}.$$

Throughout this paper we always assume that $\lambda_0 > -\infty$.

Suppose that $\lambda_0 \geq 0$, and consider the (time-independent) parabolic operator

$$Lu := \partial_t u + P(x, \partial_x)u \qquad (x, t) \in M \times (0, \infty). \tag{1.1}$$

We denote by $\mathcal{H}_P(M \times (a, b))$ the cone of all nonnegative solutions of the parabolic equation

$$Lu = 0 \qquad \text{in } M \times (a, b). \tag{1.2}$$

Let $k_P^M(x, y, t)$ be the *positive minimal heat kernel* of the parabolic operator L on the manifold M. By definition, for a fixed $y \in M$, the function $(x, t) \mapsto k_P^M(x, y, t)$ is the minimal positive solution of the equation

$$Lu = 0 \qquad \text{in } M \times (0, \infty), \tag{1.3}$$

subject to the initial data δ_y, the Dirac distribution at $y \in M$. It can be easily checked that for $\lambda \leq \lambda_0$, the heat kernel $k_{P-\lambda}^M$ of the operator $P - \lambda$ on M satisfies the identity

$$k_{P-\lambda}^M(x, y, t) = \mathrm{e}^{\lambda t} k_P^M(x, y, t). \tag{1.4}$$

So, it is enough to study the large time behavior of $k_{P-\lambda_0}^M$, and therefore, in most cases we assume that $\lambda_0(P, M) = 0$. Note that the heat kernel of the operator P^*, the formal adjoint of the operator P on M, satisfies the relation

$$k_{P^*}^M(x, y, t) = k_P^M(y, x, t).$$

Here we should mention that many authors derived upper and lower Gaussian bounds for heat kernels of elliptic operators on $M := \mathbb{R}^d$, or more generally, on noncompact Riemannian manifolds M. As a prototype result, let us recall the following classical result of Aronson [6]:

Example 1.1. Let P be a second-order uniformly elliptic operator in divergence form on $\mathbb{R}^d$ with real coefficients satisfying some general boundedness assumptions. Then the following Gaussian estimates hold:

$$C_1(4\pi t)^{-d/2}\exp\left(-C_2\frac{|x-y|^2}{t}-\omega_1 t\right)\leq k_P^{\mathbb{R}^d}(x,y,t)$$
$$\leq C_3(4\pi t)^{-d/2}\exp\left(-C_4\frac{|x-y|^2}{t}+\omega_2 t\right) \qquad \forall (x,y,t)\in\mathbb{R}^d\times\mathbb{R}^d\times\mathbb{R}_+.$$

However, since Gaussian estimates of the above type in general are not tight as $t\to\infty$, such bounds do not provide us with the exact large time behavior of the heat kernel, let alone strong ratio limits of two heat kernels.

In spite of this, and as a first and rough result concerning the large time behavior of the heat kernel, we have the following explicit and useful formula

$$\lim_{t\to\infty}\frac{\log k_P^M(x,y,t)}{t}=-\lambda_0. \tag{1.5}$$

We note that (1.5) holds in the general case, and characterizes the generalized principal eigenvalue λ_0 in terms of the large time behavior of $\log k_P^M(x,y,t)$. The above formula is well known in the symmetric case, see for example [31] and [27, Theorem 10.24]. For the proof in the general case, see Corollary 6.1.

To get a more precise result one should introduce the notion of criticality. We say that the operator P is *subcritical* (respectively, *critical*) in M if for some $x\neq y$, and therefore for any $x\neq y$, $x,y\in M$, we have

$$\int_0^\infty k_P^M(x,y,\tau)\,\mathrm{d}\tau<\infty \qquad \left(\text{respectively, } \int_0^\infty k_P^M(x,y,\tau)\,\mathrm{d}\tau=\infty\right). \tag{1.6}$$

It follows from the above definition that, roughly speaking, the heat kernel of a subcritical operator in M "decays" faster as $t\to\infty$ than the heat kernel of a critical operator in M. This rule of thumb will be discussed in Section 8.

If P is subcritical in M, then the function

$$G_P^M(x,y):=\int_0^\infty k_P^M(x,y,\tau)\,\mathrm{d}\tau \tag{1.7}$$

is called the *positive minimal Green function* of the operator P in M.

It follows from (1.5) that for $\lambda<\lambda_0$, the operator $P-\lambda$ is subcritical in M. Clearly, P is subcritical (respectively, critical) in M, if and only if P^*, is subcritical (respectively, critical) in M. Furthermore, it is well known that if P is critical in M, then $\mathcal{C}_P(M)$ is a one-dimensional cone, and any positive supersolution of the equation $Pu=0$ in M is in fact a solution. In this case, the unique positive solution $\varphi \in \mathcal{C}_P(M)$ is called *Agmon ground state* (or in short ground state) of the operator P in M [1, 48, 54]. We denote the ground state of P^* by φ^*.

The following example demonstrates two prototype behaviors as $t \to \infty$ of heat kernels corresponding to two particular classical cases.

Example 1.2.

1. Let $P = -\Delta$, $M = \mathbb{R}^d$, where $d \geq 1$. It is well known that $\lambda_0(-\Delta, \mathbb{R}^d) = 0$, and that the heat kernel is given by the Gaussian kernel. Hence,
$$\begin{aligned} e^{\lambda_0 t} k_{-\Delta}^{\mathbb{R}^d}(x, y, t) &= k_{-\Delta}^{\mathbb{R}^d}(x, y, t) \\ &= \frac{1}{(4\pi t)^{d/2}} \exp\left(\frac{-|x-y|^2}{4t}\right) \underset{t\to\infty}{\sim} t^{-d/2} \underset{t\to\infty}{\to} 0. \end{aligned}$$
So, the rate of the decay depends on the dimension, and clearly, $-\Delta$ is critical in $\mathbb{R}^d$ if and only if $d = 1, 2$. Nevertheless, the above limit is 0 in any dimension.
2. Suppose that P is a symmetric nonnegative elliptic operator with real and smooth coefficients which is defined on a smooth bounded domain $M \Subset \mathbb{R}^d$, and let $\{\varphi_n\}_{n=0}^{\infty}$ be the complete orthonormal sequence of the (Dirichlet) eigenfunctions of P with the corresponding nondecreasing sequence of eigenvalues $\{\lambda_n\}_{n=0}^{\infty}$. Then the heat kernel has the eigenfunction expansion
$$k_P^M(x, y, t) = \sum_{n=0}^{\infty} e^{-\lambda_n t} \varphi_n(x)\varphi_n(y). \tag{1.8}$$
Hence,
$$e^{\lambda_0 t} k_P^M(x, y, t) = \sum_{n=0}^{\infty} e^{(\lambda_0 - \lambda_n)t} \varphi_n(x)\varphi_n(y) \underset{t\to\infty}{\to} \varphi_0(x)\varphi_0(y) > 0.$$
Therefore, the operator $P - \lambda_0$ is critical in M, $t^{-1} \log k_{P-\lambda_0}^M(x, y, t) \underset{t\to\infty}{\to} 0$, but $k_{P-\lambda_0}^M$ does not decay as $t \to \infty$.
3. Several explicit formulas of heat kernels of certain classical operators are included in [10, 20, 27], each of which either tends to zero or converges to a positive function as $t \to \infty$.

The characterization of λ_0 in terms of the large time behavior of the heat kernel, given by (1.5), provides us with the asymptotic behavior of $\log k_P^M$ as $t \to \infty$ but not of k_P^M itself. Moreover, (1.5) does not distinguish between critical and subcritical operators. In the first part of the present article we provide a complete proof that
$$\lim_{t\to\infty} e^{\lambda_0 t} k_P^M(x, y, t)$$
always exists. This basic result has been proved in two parts in [48] and [51], and here, for the first time, we give a comprehensive and a bit simplified proof (see also [5, 12, 28, 29, 32, 54, 60, 62, 66] and references therein for previous and related results).

We have:

Theorem 1.3 ([48, 51]). *Let P be an elliptic operator defined on M, and assume that $\lambda_0(P,M) \geq 0$.*

(i) **The subcritical case:** *If $P - \lambda_0$ is subcritical in M, then*

$$\lim_{t\to\infty} \mathrm{e}^{\lambda_0 t} k_P^M(x,y,t) = 0.$$

(ii) **The positive-critical case:** *If $P - \lambda_0$ is critical in M, and the ground states φ and φ^* of $P - \lambda_0$ and $P^* - \lambda_0$, respectively, satisfy $\varphi^*\varphi \in L^1(M)$, then*

$$\lim_{t\to\infty} \mathrm{e}^{\lambda_0 t} k_P^M(x,y,t) = \frac{\varphi(x)\varphi^*(y)}{\int_M \varphi^*(z)\varphi(z)\,\mathrm{d}z}.$$

(iii) **The null-critical case:** *If $P - \lambda_0$ is critical in M, and the ground states φ and φ^* of $P - \lambda_0$ and $P^* - \lambda_0$, respectively, satisfy $\varphi^*\varphi \notin L^1(M)$, then*

$$\lim_{t\to\infty} \mathrm{e}^{\lambda_0 t} k_P^M(x,y,t) = 0.$$

Moreover, for $\lambda < \lambda_0$, let $G_{P-\lambda}^M(x,y)$ be the minimal positive Green function of the elliptic operator $P - \lambda$ on M. Then the following Abelian-Tauberian relation holds

$$\lim_{t\to\infty} \mathrm{e}^{\lambda_0 t} k_P^M(x,y,t) = \lim_{\lambda\nearrow\lambda_0} (\lambda_0 - \lambda) G_{P-\lambda}^M(x,y). \tag{1.9}$$

The outline of the present paper is as follows. In Section 2 we provide a short review of the theory of positive solutions and the basic properties of the heat kernel. The proof of Theorem 1.3 is postponed to Section 5 since it needs some preparation. It turns out that the proof of the null-critical case (given in [51]) is the most subtle part of the proof of Theorem 1.3. It relies on the large time behaviors of the parabolic capacitory potential and of the heat content that are studied in Section 3, and on an extension of Varadhan's lemma that is proved in Section 4 (see Lemma 4.1). Section 6 is devoted to some applications to Theorem 1.3. In particular, Corollary 6.7 seems to be new.

The next two sections deal with ratio limits. In Section 7, we discuss the existence of the strong ratio limit

$$\lim_{t\to\infty} \frac{k_P^M(x,y,t)}{k_P^M(x_0,x_0,t)}$$

(Davies' conjecture), and in Section 8 we deal with the conjecture that

$$\lim_{t\to\infty} \frac{k_{P_+}^M(x,y,t)}{k_{P_0}^M(x,y,t)} = 0 \qquad \forall x,y \in M, \tag{1.10}$$

where P_+ and P_0 are respectively subcritical and critical operators in M. Finally, in Section 9 we discuss the equivalence of heat kernels of two subcritical elliptic operators (with the same λ_0) that agree outside a compact set. Unlike the analogous question concerning the equivalence of Green functions, the problem concerning the equivalence of heat kernels is still "terra incognita". Solving this problem will in particular enable us to study the stability of the large time behavior of the heat kernel under perturbations.

The survey is an expanded version of a talk given by the author at the conference “Mathematical Physics, Spectral Theory and Stochastic Analysis” held in Goslar, Germany, September 11–16, 2011, in honor of Professor Michael Demuth. We note that most of the results in Sections 3–6 originally appeared in [48, 51], those of Section 7 appeared in [52], while those in Sections 8–9 originally appeared in [24].

2. Preliminaries

In this section we recall basic definitions and facts concerning the theory of nonnegative solutions of second-order linear elliptic and parabolic operators (for more details and proofs, see for example [54]).

Let P be a linear, second-order, elliptic operator defined in a noncompact, connected, C^3-smooth Riemannian manifold M of dimension d. Here P is an elliptic operator with real and Hölder continuous coefficients which in any coordinate system $(U; x_1, \ldots, x_d)$ has the form

$$P(x, \partial_x) = -\sum_{i,j=1}^{d} a_{ij}(x)\partial_i\partial_j + \sum_{i=1}^{d} b_i(x)\partial_i + c(x), \tag{2.1}$$

where $\partial_i = \partial/\partial x_i$. We assume that for every $x \in M$ the real quadratic form

$$\sum_{i,j=1}^{d} a_{ij}(x)\xi_i\xi_j, \quad \xi = (\xi_1, \ldots, \xi_d) \in \mathbb{R}^d \tag{2.2}$$

is symmetric and positive definite.

Throughout the paper we always assume that $\lambda_0(P, M) \geq 0$. In this case we simply say that the operator P is *nonnegative in* M, and write $P \geq 0$ in M. So, $P \geq 0$ in M if and only if the equation $Pu = 0$ admits a global positive solution in M. We note that in the symmetric case, by the Agmon-Allegretto-Piepenbrink theory [1], the nonnegativity of P in M is equivalent to the nonnegativity of the associated quadratic form on $C_0^\infty(M)$.

We consider the parabolic operator L

$$Lu = u_t + Pu \qquad \text{on } M \times (0, \infty), \tag{2.3}$$

and the corresponding homogeneous equation $Lu = 0$ in $M \times (0, \infty)$.

Remark 2.1. We confine ourselves mainly to classical solutions. However, since the results and the proofs throughout the paper rely on standard elliptic and parabolic regularity, and basic properties and results of potential theory, the results of the paper are also valid for weak solutions in the case where the elliptic operator P is in divergence form

$$Pu = -\sum_{i=1}^{d} \partial_i \left[\sum_{j=1}^{d} a_{ij}(x)\partial_j u + u\tilde{b_i}(x) \right] + \sum_{i=1}^{d} b_i(x)\partial_i u + c(x)u, \tag{2.4}$$

with coefficients which satisfy standard local regularity assumptions (as for example in Section 1.1 of [44]). The results are also valid in the framework of strong solutions, where the strictly elliptic operator P is of the form (2.1) and has locally bounded coefficients; the proofs differ only in minor details from the proofs given here.

We write $\Omega_1 \Subset \Omega_2$ if Ω_2 is open, $\overline{\Omega_1}$ is compact and $\overline{\Omega_1} \subset \Omega_2$. Let $f, g \in C(\Omega)$ be nonnegative functions; we use the notation $f \asymp g$ on Ω if there exists a positive constant C such that

$$C^{-1}g(x) \le f(x) \le Cg(x) \qquad \text{for all } x \in \Omega.$$

Let $\{M_j\}_{j=1}^{\infty}$ be an *exhaustion* of M, i.e., a sequence of smooth, relatively compact domains in M such that $M_1 \neq \emptyset$, $M_j \Subset M_{j+1}$ and $\cup_{j=1}^{\infty} M_j = M$. For every $j \ge 1$, we denote $M_j^* = M \setminus \mathrm{cl}(M_j)$. Let $M_\infty = M \cup \{\infty\}$ be the one-point compactification of M. By a neighborhood of infinity in M we mean a neighborhood of ∞ in M_∞, that is, a set of the form $M \setminus K$, where K is compact in M.

Assume that $P \ge 0$ in M. For every $j \ge 1$, consider the Dirichlet heat kernel $k_P^{M_j}(x, y, t)$ of the parabolic operator $L = \partial_t + P$ in M_j. So, for every continuous function f with a compact support in M, the function

$$u(x,t) := \int_{M_j} k_P^{M_j}(x, y, t) f(y)\, \mathrm{d}y$$

solves the initial-Dirichlet boundary value problems

$$\begin{aligned} Lu &= 0 \qquad \text{in } M_j \times (0, \infty), \\ u &= 0 \qquad \text{on } \partial M_j \times (0, \infty), \\ u &= f \qquad \text{on } M_j \times \{0\}. \end{aligned} \tag{2.5}$$

By the generalized maximum principle, $\{k_P^{M_j}(x, y, t)\}_{j=1}^{\infty}$ is an increasing sequence which converges to $k_P^M(x, y, t)$, the *positive minimal heat kernel* of the parabolic operator L in M.

The main properties of the positive minimal heat kernel are summarized in the following lemma.

Lemma 2.2. *Assume that $P \ge 0$ in M. The heat kernel $k_P^M(x, y, t)$ satisfies the following properties.*

1. *Positivity: $k_P^M(x, y, t) \ge 0$ for all $t \ge 0$ and $x, y \in M$.*
2. *For any $\lambda \le \lambda_0$ we have*

$$k_{P-\lambda}^M(x, y, t) = \mathrm{e}^{\lambda t} k_P^M(x, y, t). \tag{2.6}$$

3. *The heat kernel satisfies the semigroup identity*
$$\int_\Omega k_P^M(x,z,t)k_P^M(z,y,\tau)\,\mathrm{d}z = k_P^M(x,y,t+\tau) \ \ \forall t,\tau>0, \text{and } x,y\in M. \tag{2.7}$$
4. *Monotonicity: If* $M_1\subset M$*, and* $V_1\geq V_2$*, then*
$$k_P^{M_1}\leq k_P^M, \qquad \text{and} \qquad k_{P+V_1}^M\leq k_{P+V_2}^M.$$
5. *For any fixed* $y\in M$ *(respectively* $x\in M$*),* $k_P^M(x,y,t)$ *solves the equation* $u_t+P(x,\partial_x)u=0$ *(respectively* $u_t+P^*(y,\partial_y)u=0$*) in* $M\times(0,\infty)$*.*
6. *Skew product operators: Let* $M=M_1\times M_2$ *be a product of two manifolds, and denote* $x=(x_1,x_2)\in M=M_1\times M_2$*. Consider a skew product elliptic operator of the form* $P:=P_1\otimes I_2+I_1\otimes P_2$*, where* P_i *is a second-order elliptic operator on* M_i *satisfying the assumptions of the present paper, and* I_i *is the identity map on* M_i*,* $i=1,2$*. Then*
$$k_P^M(x,y,t)=k_{P_1}^{M_1}(x_1,y_1,t)k_{P_2}^{M_2}(x_2,y_2,t). \tag{2.8}$$
7. *Eigenfunction expansion: Suppose that* P *is a symmetric elliptic operator with (up to the boundary) smooth coefficients which is defined on a smooth bounded domain* M*. Let* $\{\varphi_n\}_{n=0}^\infty$ *be the complete orthonormal sequence of the (Dirichlet) eigenfunctions of* P *with the corresponding nondecreasing sequence of eigenvalues* $\{\lambda_n\}_{n=0}^\infty$*. Then the heat kernel of* P *in* M *has the eigenfunction expansion*
$$k_P^M(x,y,t)=\sum_{n=0}^\infty \mathrm{e}^{-\lambda_n t}\varphi_n(x)\varphi_n(y). \tag{2.9}$$
8. *Let* $v\in\mathcal{C}_P(M)$ *and* $v^*\in\mathcal{C}_{P^*}(M)$*. Then* [48, 49]
$$\int_M k_P^M(x,y,t)v(y)\,\mathrm{d}y\leq v(x), \quad \text{and} \quad \int_M k_P^M(x,y,t)v^*(x)\,\mathrm{d}x\leq v^*(y). \tag{2.10}$$
Moreover, (by the maximum principle) either $\int_M k_P^M(x,y,t)v(y)\,\mathrm{d}y<v(x)$ *for all* $(x,t)\in M\times(0,\infty)$*, or* $\int_M k_P^M(x,y,t)v(y)\,\mathrm{d}y=v(x)$ *for all* $(x,t)\in M\times(0,\infty)$*, and in the latter case* v *is called an* invariant solution *of the operator* P *on* M *(see for example* [21, 26, 48, 54]*).*

Remark 2.3.

1. If there exists $v\in\mathcal{C}_P(M)$ such that v is not invariant, then the positive Cauchy problem
$$Lu=0,\ u\geq 0 \quad \text{on } M\times(0,\infty), \quad u(x,0)=0 \quad x\in M$$
does not admit a unique solution.
2. An invariant solution is sometimes called *complete*. If the constant function is an invariant solution with respect to the heat operator, then one says that the heat operator *conserves probability*, and the corresponding diffusion process is said to be *stochastically complete* [27].

Definition 2.4. Let w be a positive solution of the equation $Pu = 0$ in $M \setminus K$, where $K \Subset M$. We say that w is a positive solution of the equation $Pu = 0$ of *minimal growth in a neighborhood of infinity in* M if for any $v \in C(\mathrm{cl}(M_j^*))$ which is a positive supersolution of the equation $Pu = 0$ in M_j^* for some $j \geq 1$ large enough, and satisfies $w \leq v$ on ∂M_j^*, we have $w \leq v$ in M_j^* [1, 48, 54].

In the subcritical (respectively, critical) case, the Green function $G_P^M(\cdot, y)$ (respectively, the ground state φ) is a positive solution of the equation $Pu = 0$ of minimal growth in a neighborhood of infinity in M. Recall that if $\lambda < \lambda_0$, then $P - \lambda$ is subcritical in M. In particular, if P is critical in M, then $\lambda_0 = 0$.

Next, we recall the parabolic Harnack inequality. Denote by $Q(x_0, t_0, R, \theta)$ the parabolic box

$$Q(x_0, t_0, R, \theta) := \{(x, t) \in M \times \mathbb{R} \mid \rho(x, x_0) < R, t \in (t_0, t_0 + \theta R^2)\},$$

where ρ is the given Riemannian metric on M, and $\theta > 0$. We have:

Lemma 2.5 (Harnack inequality). *Let u be a nonnegative solution of the equation $Lu = 0$ in $Q(x_0, t_0, R, \theta)$, and assume that $\theta > 1$ and $0 < R < R_0$. Then*

$$u(x_0, t_0 + R^2) \leq Cu(x, t_0 + \theta R^2) \tag{2.11}$$

for every $\rho(x, x_0) < R/2$, where $C = C(L, d, R_0, \theta)$. Moreover, C varies within bounded bounds for all $\theta > 1$ such that $0 < \varepsilon \leq (\theta - 1)^{-1} \leq M$.

Let $v \in \mathcal{C}_P(M)$ and $v^* \in \mathcal{C}_{P^*}(M)$. Then the parabolic Harnack inequality (2.11), and (2.10) imply the following important estimate

$$k_P^M(x, y, t) \leq c_1(y) v(x), \qquad \text{and } k_P^M(x, y, t) \leq c_2(x) v^*(y) \tag{2.12}$$

for all $x, y \in M$ and $t > 1$ (see [48, (3.29–30)]). Recall that in the critical case, by uniqueness, v and v^* are (up to a multiplicative constant) the ground states φ and φ^* of P and P^* respectively. Moreover, it is known that the ground state φ (respectively, φ^*) is a positive invariant solution of the operator P (respectively, P^*) in M. So,

$$\int_M k_P^M(x, y, t)\varphi(y)\,\mathrm{d}y = \varphi(x), \text{ and } \int_M k_P^M(x, y, t)\varphi^*(x)\,\mathrm{d}x = \varphi^*(y). \tag{2.13}$$

We distinguish between two types of criticality.

Definition 2.6. A critical operator P is said to be *positive-critical* in M if $\varphi^*\varphi \in L^1(M)$, and *null-critical* in M if $\varphi^*\varphi \not\in L^1(M)$.

Remark 2.7. Let $\mathbf{1}$ be the constant function on M, taking at any point $x \in M$ the value 1. Suppose that $P\mathbf{1} = 0$. Then P is subcritical (respectively, positive-critical, null-critical) in M if and only if the corresponding diffusion process is transient (respectively, positive-recurrent, null-recurrent). For a thorough discussion of the probabilistic interpretation of criticality theory, see [54].

In fact, in the critical case it is natural to use the well-known (Doob) h-transform with $h=\varphi$, where φ is the ground state of P. So,

$$P^{\varphi}u := \frac{1}{\varphi}P(\varphi u) \quad \text{and therefore} \quad k_{P^{\varphi}}^{M}(x,y,t) = \frac{1}{\varphi(x)}k_{P}^{M}(x,y,t)\varphi(y).$$

Clearly, P^{φ} is an elliptic operator which satisfies all our assumptions. Note that P^{φ} is null-critical (respectively, positive-critical) if and only if P is null-critical (respectively, positive-critical), and the ground states of P^{φ} and $(P^{\varphi})^{*}$ are $\mathbf{1}$ and $\varphi^{*}\varphi$, respectively. Moreover,

$$\lim_{t\to\infty} k_{P^{\varphi}}^{M}(x,y,t) = 0 \quad \text{if and only if} \quad \lim_{t\to\infty} k_{P}^{M}(x,y,t) = 0.$$

Therefore, in the critical case, we may assume that

$$P\mathbf{1}=0, \text{ and } P \text{ is a critical operator in } M. \tag{\textbf{A}}$$

It is well known that on a general noncompact manifold M, the solution of the Cauchy problem for the parabolic equation $Lu=0$ is not uniquely determined (see for example [30] and the references therein). On the other hand, under Assumption **(A)**, there is a unique *minimal* solution of the Cauchy problem and of certain initial-boundary value problems for *bounded* initial and boundary conditions. More precisely,

Definition 2.8. Assume that $P\mathbf{1}=0$. Let f be a *bounded* continuous function on M. By the *minimal solution* u of the Cauchy problem

$$\begin{aligned} Lu &= 0 \quad \text{in } M\times(0,\infty),\\ u &= f \quad \text{on } M\times\{0\}, \end{aligned}$$

we mean the function

$$u(x,t) := \int_M k_P^M(x,y,t) f(y)\,\mathrm{d}y. \tag{2.14}$$

Note that (2.10) implies that u in (2.14) is well defined.

Definition 2.9. Assume that $P\mathbf{1}=0$. Let $B \Subset M_1$ be a smooth bounded domain such that $B^{*} := M\setminus \mathrm{cl}(B)$ is connected. Assume that f is a bounded continuous function on B^{*}, and g is a bounded continuous function on $\partial B\times(0,\infty)$. By the *minimal solution* u of the initial-boundary value problem

$$\begin{aligned} Lu &= 0 \quad \text{in } B^{*}\times(0,\infty),\\ u &= g \quad \text{on } \partial B\times(0,\infty),\\ u &= f \quad \text{on } B^{*}\times\{0\}, \end{aligned} \tag{2.15}$$

we mean the limit of the solutions u_j of the following initial-boundary value problems

$$\begin{aligned} Lu &= 0 \quad \text{in } (B^{*}\cap M_j)\times(0,\infty),\\ u &= g \quad \text{on } \partial B\times(0,\infty),\\ u &= 0 \quad \text{on } \partial M_j\times(0,\infty),\\ u &= f \quad \text{on } (B^{*}\cap M_j)\times\{0\}. \end{aligned}$$

Remark 2.10. It can be easily checked that the sequence $\{u_j\}$ is indeed a converging sequence which converges to a solution of the initial-boundary value problem (2.15).

Next, we recall some results concerning the theory of positive solutions of *elliptic* equations that we shall need in the sequel.

The first result is a *Liouville comparison theorem* in the symmetric case.

Theorem 2.11 ([53]). *Let P_0 and P_1 be two symmetric operators of the form*

$$P_j u = -m_j^{-1}\operatorname{div}(m_j A_j \nabla u) + V_j u \qquad j = 0, 1, \tag{2.16}$$

defined on $L^2(M, m_0\,\mathrm{d}x)$ and $L^2(M, m_1\,\mathrm{d}x)$, respectively.

Assume that the following assumptions hold true.

(i) *The operator P_0 is critical in M. Denote by $\varphi \in \mathcal{C}_{P_0}(M)$ its ground state.*
(ii) *$P_1 \geq 0$ in M, and there exists a real function $\psi \in H^1_{\mathrm{loc}}(M)$ such that $\psi_+ \neq 0$, and $P_1\psi \leq 0$ in M, where $u_+(x) := \max\{0, u(x)\}$.*
(iii) *The following matrix inequality holds*

$$(\psi_+)^2(x) m_1(x) A_1(x) \leq C\varphi^2(x) m_0(x) A_0(x) \qquad \text{for a.e. } x \in M, \tag{2.17}$$

where $C > 0$ is a positive constant.

Then the operator P_1 is critical in M, and ψ is its ground state. In particular, $\dim \mathcal{C}_{P_1}(M) = 1$ and $\lambda_0(P_1, M) = 0$.

In the sequel we shall also need to use results concerning small and semismall perturbations of a subcritical elliptic operator. These notions were introduced in [46] and [43] respectively, and are closely related to the stability of $\mathcal{C}_P(\Omega)$ under perturbation by a potential V.

Definition 2.12. Let P be a subcritical operator in M, and let V be a real-valued potential defined on M.

(i) We say that V is a *small perturbation* of P in M if

$$\lim_{j\to\infty}\left\{\sup_{x,y\in M_j^*}\int_{M_j^*}\frac{G_P^M(x,z)|V(z)|G_P^M(z,y)}{G_P^M(x,y)}\,\mathrm{d}z\right\} = 0. \tag{2.18}$$

(ii) V is a *semismall perturbation* of P in M if for some $x_0 \in M$ we have

$$\lim_{j\to\infty}\left\{\sup_{y\in M_j^*}\int_{M_j^*}\frac{G_P^M(x_0,z)|V(z)|G_P^M(z,y)}{G_P^M(x_0,y)}\,\mathrm{d}z\right\} = 0. \tag{2.19}$$

Recall that small perturbations are semismall [43]. For semismall perturbations we have

Theorem 2.13 ([43, 46, 47]). *Let P be a subcritical operator in M. Assume that $V = V_+ - V_-$ is a semismall perturbation of P^* in M satisfying $V_- \neq 0$, where $V_\pm(x) = \max\{0, \pm V(x)\}$.*

Then there exists $\alpha_0 > 0$ such that $P_\alpha := P + \alpha V$ is subcritical in M for all $0 \leq \alpha < \alpha_0$ and critical for $\alpha = \alpha_0$.

Moreover, let φ be the ground state of $P+\alpha_0 V$ and let y_0 be a fixed reference point in M_1. Then for any $0 \le \alpha < \alpha_0$

$$\varphi \asymp G^M_{P_\alpha}(\cdot, y_0) \qquad \text{in } M_1^*,$$

where the equivalence constant depends on α.

3. Capacitory potential and heat content

Our first result concerning the large time behavior of positive solutions is given by the following simple lemma that does not distinguish between null-critical and positive-critical operators.

Lemma 3.1. *Assume that $P\mathbf{1} = 0$ and that P is critical in M. Let $B := B(x_0, \delta) \subset\subset M$ be the ball of radius δ centered at x_0, and suppose that $B^* = M \setminus \mathrm{cl}(B)$ is connected. Let w be* **the heat content of** *B^*, i.e., the minimal nonnegative solution of the following initial-boundary value problem*

$$\begin{aligned} Lu &= 0 \qquad \text{in } B^* \times (0,\infty),\\ u &= 0 \qquad \text{on } \partial B \times (0,\infty),\\ u &= 1 \qquad \text{on } B^* \times \{0\}. \end{aligned} \tag{3.1}$$

Then w is a decreasing function of t, and $\lim_{t\to\infty} w(x,t) = 0$ locally uniformly in B^*.

Proof. Clearly,

$$w(x,t) = \int_{B^*} k_P^{B^*}(x,y,t)\,\mathrm{d}y < \int_M k_P^M(x,y,t)\,\mathrm{d}y = 1. \tag{3.2}$$

It follows that $0 < w < 1$ in $B^* \times (0,\infty)$. Let $\varepsilon > 0$. By the semigroup identity and (3.2),

$$\begin{aligned} w(x,t+\varepsilon) &= \int_{B^*} k_P^{B^*}(x,y,t+\varepsilon)\,\mathrm{d}y = \int_{B^*}\left(\int_{B^*} k_P^{B^*}(x,z,t)k_P^{B^*}(z,y,\varepsilon)\,\mathrm{d}z\right)\mathrm{d}y\\ &= \int_{B^*} k_P^{B^*}(x,z,t)\left(\int_{B^*} k_P^{B^*}(z,y,\varepsilon)\,\mathrm{d}y\right)\mathrm{d}z\\ &< \int_{B^*} k_P^{B^*}(x,z,t)\,\mathrm{d}z = w(x,t). \end{aligned} \tag{3.3}$$

Hence, w is a decreasing function of t, and therefore, $\lim_{t\to\infty} w(x,t)$ exists. We denote $v(x) := \lim_{t\to\infty} w(x,t)$. Note that the above argument shows that even in the subcritical case w is a decreasing function of t.

For $\tau > 0$, consider the function $\nu(x,t;\tau) := w(x,t+\tau)$, where $t > -\tau$. Then $\nu(x,t;\tau)$ is a nonnegative solution of the parabolic equation $Lu = 0$ in $B^* \times (-\tau,\infty)$ which satisfies $u = 0$ on $\partial B \times (-\tau,\infty)$. By a standard parabolic argument as $\tau \to \infty$, any converging subsequence of this set of solutions converges locally uniformly to a solution of the parabolic equation $Lu = 0$ in $B^* \times \mathbb{R}$ which satisfies $u = 0$ on $\partial B \times \mathbb{R}$. Since $\lim_{\tau\to\infty} \nu(x,t;\tau) = \lim_{\tau\to\infty} w(x,\tau) = v(x)$, the limit does not depend on t, and v is a solution of the elliptic equation $Pu = 0$ in B^*, and satisfies $v = 0$ on ∂B. Furthermore, $0 \leq v < \mathbf{1}$.

Therefore, $\mathbf{1} - v$ is a positive solution of the equation $Pu = 0$ in B^* which satisfies $u = 1$ on ∂B. On the other hand, it follows from the criticality assumption that $\mathbf{1}$ is the minimal positive solution of the equation $Pu = 0$ in B^* which satisfies $u = 1$ on ∂B. Thus, $\mathbf{1} \leq \mathbf{1} - v$, and therefore, $v = 0$. □

Definition 3.2. Let $B := B(x_0, \delta) \subset\subset M$. Suppose that $B^* = M \setminus \mathrm{cl}(B)$ is connected. The nonnegative (minimal) solution

$$v(x,t) = \mathbf{1} - \int_{B^*} k_P^{B^*}(x,y,t)\,\mathrm{d}y$$

is called the *parabolic capacitory potential of* B^*. Note that v is indeed the minimal nonnegative solution of the initial-boundary value problem

$$\begin{aligned} Lu &= 0 \quad \text{in } B^* \times (0,\infty),\\ u &= 1 \quad \text{on } \partial B \times (0,\infty),\\ u &= 0 \quad \text{on } B^* \times \{0\}. \end{aligned} \tag{3.4}$$

Corollary 3.3. *Under the assumptions of Lemma* 3.1*, the parabolic capacitory potential* v *of* B^* *is an increasing function of* t*, and* $\lim_{t\to\infty} v(x,t) = 1$ *locally uniformly in* B^**.*

Proof. Using an exhaustion argument it is easily verified that

$$v(x,t) = \mathbf{1} - \int_{B^*} k_P^{B^*}(x,y,t)\,\mathrm{d}y = \mathbf{1} - w(x,t), \tag{3.5}$$

where w is the heat content of B^*. Therefore, the corollary follows directly from Lemma 3.1. □

4. Varadhan's lemma

Varadhan's celebrated lemma (see, [62, Lemma 9, p. 259] or [54, pp. 192–193]) deals with the large time behavior of minimal solutions of the Cauchy problem with *bounded* initial data (assuming that $P\mathbf{1} = 0$). It turns out that the limit as $t \to \infty$ of such solutions might not exist, but, under further conditions, the spacial oscillation of the solution tends to zero as $t \to \infty$. In the present section we slightly extend Varadhan's lemma (Lemma 4.1). This extended version of the lemma is crucially used in the proof of the null-critical case in Theorem 1.3.

Varadhan proved his lemma for *positive-critical* operators on $\mathbb{R}^d$ using a purely probabilistic approach (ours is purely analytic). Our key observation is that the assertion of Varadhan's lemma is valid in our general setting under the weaker assumption that the skew product operator $\bar{P} := P \otimes I + I \otimes P$ is critical in $\bar{M} := M \times M$, where I is the identity operator on M. Note that if $\bar{P}$ is critical in $\bar{M}$, then P is critical in M. On the other hand, if P is positive-critical in M, then $\bar{P}$ is positive-critical in $\bar{M}$. Moreover, if $\bar{P}$ is subcritical in $\bar{M}$, then by part

(i) of Theorem 1.3, the heat kernel of $\bar{P}$ on $\bar{M}$ tends to zero as $t \to \infty$. Since the heat kernel of $\bar{P}$ is equal to the product of the heat kernels of its factors (see Lemma 2.2), it follows that if $\bar{P}$ is subcritical in $\bar{M}$, then $\lim_{t\to\infty} k_P^M(x,y,t) = 0$.

Consider the Riemannian product manifold $\bar{M} = M \times M$. A point in $\bar{M}$ is denoted by $\bar{x} = (x_1, x_2)$. By P_{x_i}, $i = 1, 2$, we denote the operator P in the variable x_i. So, $\bar{P} = P_{x_1} + P_{x_2}$ is in fact the above skew product operator defined on $\bar{M}$. We denote by $\bar{L}$ the corresponding parabolic operator.

Lemma 4.1 (Varadhan's lemma [51]). *Assume that* $P\mathbf{1} = 0$. *Suppose further that* $\bar{P}$ *is critical on* $\bar{M}$. *Let* f *be a continuous bounded function on* M, *and let*

$$u(x,t) = \int_M k_P^M(x,y,t) f(y)\,\mathrm{d}y$$

be the minimal solution of the Cauchy problem with initial data f *on* M. *Fix* $K \subset\subset M$. *Then*

$$\lim_{t\to\infty} \sup_{x_1,x_2\in K} |u(x_1,t) - u(x_2,t)| = 0.$$

Proof. Denote by $\bar{u}(\bar{x},t) := u(x_1,t) - u(x_2,t)$. Recall that the heat kernel $\bar{k}(\bar{x},\bar{y},t)$ of the operator $\bar{L}$ on $\bar{M}$ satisfies

$$\bar{k}_{\bar{P}}^{\bar{M}}(\bar{x},\bar{y},t) = k_P^M(x_1,y_1,t) k_P^M(x_2,y_2,t). \tag{4.1}$$

By (2.13) and (4.1), we have

$$\begin{aligned}
\bar{u}(\bar{x},t) &= u(x_1,t) - u(x_2,t) \\
&= \int_M k_P^M(x_1,y_1,t) f(y_1)\,\mathrm{d}y_1 - \int_M k_P^M(x_2,y_2,t) f(y_2)\,\mathrm{d}y_2 \\
&= \int_M \int_M k_P^M(x_1,y_1,t) k_P^M(x_2,y_2,t)(f(y_1) - f(y_2))\,\mathrm{d}y_1\,\mathrm{d}y_2 \\
&= \int_{\bar{M}} \bar{k}_{\bar{P}}^{\bar{M}}(\bar{x},\bar{y},t)(f(y_1) - f(y_2))\,\mathrm{d}\bar{y}.
\end{aligned}$$

Hence, $\bar{u}$ is the minimal solution of the Cauchy problem for the equation $\bar{L}\bar{w} = 0$ on $\bar{M} \times (0,\infty)$ with the bounded initial data $\bar{f}(\bar{x}) := f(x_1) - f(x_2)$, where $\bar{x} \in \bar{M}$.

Fix a compact set $K \subset\subset M$ and $x_0 \in M \setminus K$, and let $\varepsilon > 0$. Let $B := B((x_0,x_0),\delta) \subset\subset \bar{M} \setminus \bar{K}$, where $\bar{K} = K \times K$, and δ will be determined below. We may assume that $B^* = \bar{M} \setminus \mathrm{cl}(B)$ is connected. Then $\bar{u}$ is a minimal solution of the following initial-boundary value problem

$$\begin{aligned}
\bar{L}\bar{u} &= 0 && \text{in } B^* \times (0,\infty), \\
\bar{u}(\bar{x},t) &= u(x_1,t) - u(x_2,t) && \text{on } \partial B \times (0,\infty), \\
\bar{u}(\bar{x},0) &= f(x_1) - f(x_2) && \text{on } B^* \times \{0\}.
\end{aligned} \tag{4.2}$$

We need to prove that $\lim_{t\to\infty} \bar{u}(\bar{x},t) = 0$.

By the superposition principle (which obviously holds for minimal solutions), we have

$$\bar{u}(\bar{x},t) = u_1(\bar{x},t) + u_2(\bar{x},t) \qquad \text{on } B^* \times [1,\infty),$$

where u_1 solves the initial-boundary value problem

$$\begin{aligned} \bar{L}u_1 &= 0 && \text{in } B^* \times (1,\infty), \\ u_1(\bar{x},t) &= u(x_1,t) - u(x_2,t) && \text{on } \partial B \times (1,\infty), \\ u_1(\bar{x},0) &= 0 && \text{on } B^* \times \{1\}, \end{aligned} \tag{4.3}$$

and u_2 solves the initial-boundary value problem

$$\begin{aligned} \bar{L}u_2 &= 0 && \text{in } B^* \times (1,\infty), \\ u_2(\bar{x},t) &= 0 && \text{on } \partial B \times (1,\infty), \\ u_2(\bar{x},0) &= u(x_1,1) - u(x_2,1) && \text{on } B^* \times \{1\}. \end{aligned} \tag{4.4}$$

Clearly, $|\bar{u}(\bar{x},t)| \leq 2\|f\|_\infty$ on $\bar{M} \times (0,\infty)$. Note that if $\bar{x} = (x_1,x_2) \in \partial B$, then on M, $\mathrm{dist}_M(x_1,x_2) \leq 2\delta$. Using Schauder's parabolic interior estimates on M, it follows that if δ is small enough, then

$$|\bar{u}(\bar{x},t)| = |u(x_1,t) - u(x_2,t)| < \varepsilon \quad \text{on } \partial B \times (1,\infty).$$

By comparison of u_1 with the parabolic capacitory potential of B^*, we obtain that

$$|u_1(\bar{x},t)| \leq \varepsilon \left(1 - \int_{B^*} \bar{k}_{\bar{P}}^{B^*}(\bar{x},\bar{y},t-1)\,\mathrm{d}\bar{y}\right) < \varepsilon \qquad \text{in } B^* \times (1,\infty). \tag{4.5}$$

On the other hand,

$$|u_2(\bar{x},t)| \leq 2\|f\|_\infty \int_{B^*} \bar{k}_{\bar{P}}^{B^*}(\bar{x},\bar{y},t-1)\,\mathrm{d}\bar{y} \qquad \text{in } B^* \times (1,\infty). \tag{4.6}$$

It follows from (4.6) and Lemma 3.1 that there exists $T > 0$ such that

$$|u_2(\bar{x},t)| \leq \varepsilon \quad \text{for all } \bar{x} \in \bar{K} \text{ and } t > T. \tag{4.7}$$

Combining (4.5) and (4.7), we obtain that $|u(x_1,t) - u(x_2,t)| \leq 2\varepsilon$ for all $x_1, x_2 \in K$ and $t > T$. Since ε is arbitrary, the lemma is proved. □

5. Existence of $\lim_{t\to\infty} \mathrm{e}^{\lambda_0 t} k_P^M(x,y,t)$

The present section is devoted to the proof of Theorem 1.3 which claims that $\lim_{t\to\infty} \mathrm{e}^{\lambda_0 t} k_P^M(x,y,t)$ always exists. Without loss of generality, we may assume that $\lambda_0 = 0$. For convenience, we denote by k the heat kernel k_P^M of the operator P in M.

Proof of Theorem 1.3. (i) *The subcritical case*: Suppose that P is subcritical in Ω. It means that for any $x, y, \in M$ we have

$$\int_1^\infty k(x,y,t)\,\mathrm{d}t < \infty. \tag{5.1}$$

Let $x, y \in \Omega$ be fixed, and suppose that $k(x,y,t)$ does not converge to zero as $t \to \infty$. Then there exist an increasing sequence $t_j \to \infty$, $t_{j+1} - t_j > 1$, and $\varepsilon > 0$, such that $k(x,y,t_j) > \varepsilon$ for all $j > 1$. Using the parabolic Harnack inequality

(2.11), we deduce that there exists $C > 0$ (C may depend on x, y, Ω, and P) such that

$$\int_{t_j}^{t_{j+1}} k(x,y,t)\,\mathrm{d}t > C\varepsilon \qquad \forall j > 2. \tag{5.2}$$

But this contradicts (5.1).

(ii) *The positive-critical case*: Let P be a critical operator in M and let $\{t_j\}_{j=1}^{\infty} \subset \mathbb{R}$ be a sequence such that $t_j \to \infty$, and define:

$$u_j(x,y,t) = k(x,y,t+t_j).$$

Fix $x_0, y_0 \in M$. By (2.12) we have

$$u_j(x,y_0,t) \le c_1(y_0)\varphi(x), \qquad \Big(u_j(x_0,y,t) \le c_2(x_0)\varphi^*(y),\Big) \tag{5.3}$$

for all $x \in M$ ($y \in M$) and $t \in \mathbb{R}$ and $j > J(t)$. Using the parabolic Harnack inequality and a standard Parabolic regularity argument we may subtract a subsequence of $\{u_j\}$ (which we rename by $\{u_j\}$) that converges locally uniformly to a nonnegative solution $u(x,y,t)$ of the parabolic equations

$$Lu = \partial_t u + P(x,\partial_x)u = 0, \quad Lu = \partial_t u + P(y,\partial_y)u = 0 \quad \text{ in } M \times \mathbb{R}.$$

Moreover, u satisfies the estimates

$$u(x,y_0,t) \le c_1(y_0)\varphi(x) \qquad \forall (x,t) \in M \times \mathbb{R}, \tag{5.4}$$

$$u(x_0,y,t) \le c_2(x_0)\varphi^*(y) \qquad \forall (y,t) \in M \times \mathbb{R}. \tag{5.5}$$

Using the semigroup property we have for all $t, \tau > 0$

$$\begin{aligned}\int_M k(x,z,\tau)k(z,y,t+t_j)\,\mathrm{d}z &= \int_M k(x,z,t+t_j)k(z,y,\tau)\,\mathrm{d}z \\ &= k(x,y,\tau+t+t_j)\end{aligned} \tag{5.6}$$

for all $j \ge 1$. On the other hand, by (2.13), the ground state φ is a positive invariant solution. Consequently, for any $x \in M$ and $\tau > 0$, $k(x,\cdot,\tau)\varphi \in L^1(M)$. Similarly, for all $\tau > 0$ and $y \in M$, $\varphi^* k(\cdot,y,\tau) \in L^1(M)$. Hence, by estimates (5.3) and the Lebesgue dominated convergence theorem, we obtain

$$\int_M k(x,z,\tau)u(z,y,t)\,\mathrm{d}z = \int_M u(x,z,t)k(z,y,\tau)\,\mathrm{d}z = u(x,y,\tau+t), \tag{5.7}$$

where $u(x,y,t) = \lim_{j\to\infty} k(x,y,t+t_j)$. In particular, for $\tau = t_j$ and $t = -t_j$ we have

$$\int_M k(x,z,t_j)u(z,y,-t_j)\,\mathrm{d}z = \int_M u(x,z,-t_j)k(z,y,t_j)\,\mathrm{d}z = u(x,y,0) \tag{5.8}$$

Invoking again estimates (2.12), and (5.4)–(5.5), we see that the integrands in (5.8) are bounded by $C(x,y)\varphi(z)\varphi^*(z)$. Recall our assumption that $\varphi(x)\varphi^*(x) \in L^1(M)$, hence, the Lebesgue dominated convergence theorem implies

$$\int_M u(x,z,0)\hat{u}(z,y,0)\,\mathrm{d}z = \int_M \hat{u}(x,z,0)u(z,y,0)\,\mathrm{d}z = u(x,y,0), \tag{5.9}$$

where

$$\hat{u}(x,y,t) := \lim_{j\to\infty} u(x,y,t-t_j), \tag{5.10}$$

and again we may assume that the limit in (5.10) exists.

On the other hand, by the invariance property (2.13), and estimates (2.12), we get

$$\int_M u(x,z,\tau)\varphi(z)\,\mathrm{d}z = \varphi(x), \qquad \int_M \varphi^*(z)u(z,y,t)\,\mathrm{d}z = \varphi^*(y). \tag{5.11}$$

In particular $u(x,y,t) > 0$. It follows from the Harnack inequality and (5.9) that $\hat{u}(x,y,t)$ is also positive and we have

$$\int_M \int_M \hat{u}(x,z,0)u(z,y,0)\,\mathrm{d}z\varphi(y)\,\mathrm{d}y = \int_M u(x,y,0)\varphi(y)\,\mathrm{d}y. \tag{5.12}$$

Consequently, (5.11) and (5.12) imply that

$$\int_M \hat{u}(x,z,0)\varphi(z)\,\mathrm{d}z = \varphi(x). \tag{5.13}$$

Define integral operators

$$Uf(x) := \int_M \hat{u}(x,z,0)f(z)\,\mathrm{d}z, \qquad U^*f(y) := \int_M \hat{u}(z,y,0)f(z)\,\mathrm{d}z. \tag{5.14}$$

By (5.9) and (5.13) we see that $\varphi(x)$ and $u(x,y,0)$ (as a function of x) are positive eigenfunctions of the operator U with an eigenvalue 1, and for every $x \in M$, $u(x,y,0)$ is a positive eigenfunction of U^* with an eigenvalue 1. Moreover, for every $x \in M$, $u(x,\cdot,0)\varphi \in L^1(M)$ and for every $x,z \in M$, $u(x,\cdot,0)u(\cdot,z,0) \in L^1(M)$. Consequently, it follows [48, Lemma 3.4] that 1 is a simple eigenvalue of the integral operator U. Hence,

$$u(x,y,0) = \beta(y)\varphi(x). \tag{5.15}$$

By (5.11) and (5.15) we have

$$\int_M \varphi^*(z)\beta(y)\varphi(z)\,\mathrm{d}z = \int_M \varphi^*(z)u(z,y,0)\,\mathrm{d}z = \varphi^*(y). \tag{5.16}$$

Therefore, we obtain from (5.15) and (5.16) that $\beta(y) = \frac{\varphi^*(y)}{\int_M \varphi(z)\varphi^*(z)\,\mathrm{d}z}$.

Thus,

$$\lim_{j\to\infty} k(x,y,t_j) = u(x,y,0) = \frac{\varphi(x)\varphi^*(y)}{\int_M \varphi(z)\varphi^*(z)\,\mathrm{d}z}\,, \tag{5.17}$$

and the positive-critical case is proved since the limit in (5.17) is independent of the sequence $\{t_j\}$.

(iii) *The null-critical case*: Without loss of generality, we may assume that $P\mathbf{1} = 0$, where P is a null-critical operator in M. We need to prove that

$$\lim_{t\to\infty} k_P^M(x,y,t) = 0.$$

As in Lemma 4.1 (Varadhan's lemma), consider the Riemannian product manifold $\bar{M} := M \times M$, and let $\bar{P} = P_{x_1} + P_{x_2}$ be the corresponding skew product operator which is defined on $\bar{M}$.

If $\bar{P}$ is subcritical on $\bar{M}$, then by part (i), $\lim_{t\to\infty} \bar{k}_{\bar{P}}^{\bar{M}}(\bar{x}, \bar{y}, t) = 0$, and since

$$\bar{k}_{\bar{P}}^{\bar{M}}(\bar{x}, \bar{y}, t) = k_P^M(x_1, y_1, t) k_P^M(x_2, y_2, t),$$

it follows that $\lim_{t\to\infty} k_P^M(x, y, t) = 0$.

Therefore, there remains to prove the theorem for the case where $\bar{P}$ is critical in $\bar{M}$. Fix a nonnegative, bounded, continuous function $f \neq 0$ such that $\varphi^* f \in L^1(M)$, and consider the solution

$$v(x, t) := \int_M k_P^M(x, y, t) f(y)\,\mathrm{d}y.$$

Let $t_n \to \infty$, and consider the sequence $\{v_n(x, t) := v(x, t + t_n)\}$. As in part (ii), up to a subsequence, $\{v_n\}$ converges to a nonnegative solution $u \in \mathcal{H}_P(M \times \mathbb{R})$.

Invoking Lemma 4.1 (Varadhan's lemma), we see that $u(x, t) = \alpha(t)$. Since u solves the parabolic equation $Lu = 0$, it follows that $\alpha(t)$ is a nonnegative constant α.

We claim that $\alpha = 0$. Suppose to the contrary that $\alpha > 0$. The assumption that $\varphi^* f \in L^1(M)$ and (2.13) imply that for any $t > 0$

$$\begin{aligned} \int_M \varphi^*(y) v(y, t)\,\mathrm{d}y &= \int_M \varphi^*(y) \left(\int_M k_P^M(y, z, t) f(z)\,\mathrm{d}z \right) \mathrm{d}y \\ &= \int_M \left(\int_M \varphi^*(y) k_P^M(y, z, t)\,\mathrm{d}y \right) f(z)\,\mathrm{d}z = \int_M \varphi^*(z) f(z)\,\mathrm{d}z < \infty. \end{aligned} \tag{5.18}$$

On the other hand, by the null-criticality, Fatou's lemma, and (5.18) we have

$$\begin{aligned} \infty = \int_M \varphi^*(z) \alpha\,\mathrm{d}z &= \int_M \varphi^*(z) \lim_{n\to\infty} v(z, t_n)\,\mathrm{d}z \\ &\leq \liminf_{n\to\infty} \int_M \varphi^*(z) v(z, t_n)\,\mathrm{d}z = \int_M \varphi^*(z) f(z)\,\mathrm{d}z < \infty. \end{aligned}$$

Hence $\alpha = 0$, and therefore

$$\lim_{t\to\infty} \int_M k_P^M(x, y, t) f(y)\,\mathrm{d}y = \lim_{t\to\infty} v(x, t) = 0. \tag{5.19}$$

Now fix $y \in M$ and let $f := k_P^M(\cdot, y, 1)$. Consider the minimal solution of the Cauchy problem with initial data f. So, by the semigroup property we have

$$u(x, t) := \int_M k_P^M(x, z, t) f(z)\,\mathrm{d}z = \int_M k_P^M(x, z, t) k_P^M(z, y, 1)\,\mathrm{d}z = k_P^M(x, y, t + 1).$$

In view of (2.12) (with $v = \mathbf{1}$) and (2.13), the function f is bounded and satisfies $f\varphi^* \in L^1(M)$. Therefore, by (5.19) $\lim_{t\to\infty} u(x, t) = 0$. Thus,

$$\lim_{t\to\infty} k_P^M(x, y, t) = \lim_{t\to\infty} k_P^M(x, y, t + 1) = \lim_{t\to\infty} u(x, t) = 0.$$

The last statement of the theorem concerning the behavior of the Green function $G^M_{P-\lambda}(x,y)$ as $\lambda \to \lambda_0$ follows from the first part of the theorem using a classical Abelian theorem [58, Theorem 10.2]. □

6. Applications of Theorem 1.3

We discuss in this section some applications of Theorem 1.3 and comment on related results. First we prove (1.5), which characterizes λ_0 in terms of the large time behavior of $\log k_P^M(x,y,t)$.

Corollary 6.1 ([24]). *The heat kernel satisfies*

$$\lim_{t\to\infty} \frac{\log k_P^M(x,y,t)}{t} = -\lambda_0(P,M) \qquad x,y \in M. \tag{6.1}$$

Proof. The needed upper bound for the validity of (6.1) follows directly from Theorem 1.3 and (1.4).

The lower bound is obtained by a standard exhaustion argument and Theorem 1.3 (cf. the proof of [27, Theorem 10.24]). Indeed, let $\{M_j\}_{j=1}^\infty$ be an *exhaustion* of M. Recall that since M_j is a smooth bounded domain, the operator $P - \lambda_0(P, M_j)$ is positive-critical in M_j. Therefore, Theorem 1.3, and the monotonicity of heat kernels with respect to domains (see part 4 of Lemma 2.2) imply that

$$\liminf_{t\to\infty} \frac{\log k_P^M(x,y,t)}{t} \geq \lim_{t\to\infty} \frac{\log k_P^{M_j}(x,y,t)}{t} = -\lambda_0(P,M_j).$$

Since $\lim_{j\to\infty} \lambda_0(P,M_j) = \lambda_0(P,M)$, we obtain the needed lower bound. □

We now use Theorem 1.3 to strengthen Lemma 4.1. More precisely, in the following result we obtain the large time behavior of solutions of the Cauchy problem with initial conditions which satisfy a certain (and in some sense optimal) integrability condition.

Corollary 6.2 ([51]). *Let P be an elliptic operator of the form* (2.1) *such that $\lambda_0 \geq 0$. Let f be a continuous function on M such that $v^* f \in L^1(M)$ for some $v^* \in \mathcal{C}_{P^*}(M)$. Let*

$$u(x,t) = \int_M k_P^M(x,y,t) f(y)\,\mathrm{d}y$$

be the minimal solution of the Cauchy problem with initial data f on M. Fix $K \subset\subset M$. Then

$$\lim_{t\to\infty} \sup_{x\in K} |u(x,t) - \mathcal{F}(x)| = 0,$$

where

$$\mathcal{F}(x) := \begin{cases} \dfrac{\int_M f(y)\varphi^*(y)\,\mathrm{d}y}{\int_M \varphi(y)\varphi^*(y)\,\mathrm{d}y}\,\varphi(x) & \text{if } P \text{ is positive-critical in } M, \\ 0 & \text{otherwise.} \end{cases}$$

Proof. Since $v^* f \in L^1(M)$, estimate (2.12), and the dominated convergence theorem imply that

$$\lim_{t\to\infty} u(x,t) = \lim_{t\to\infty} \int_M k_P^M(x,y,t) f(y)\,\mathrm{d}y = \int_M \lim_{t\to\infty} \left[k_P^M(x,y,t) f(y)\right] \mathrm{d}y,$$

and the claim of the corollary follows from Theorem 1.3. □

Assume now that $P\mathbf{1} = 0$ and $\int_M k_P^M(\cdot,y,t)\,\mathrm{d}y = \mathbf{1}$ (i.e., $\mathbf{1}$ is a positive invariant solution of the operator P in M). Corollary 6.2 implies that for any $j \geq 1$ and all $x \in M$ we have

$$\lim_{t\to\infty} \int_{M_j^*} k_P^M(x,y,t)\,\mathrm{d}y = \begin{cases} \dfrac{\int_{M_j^*} \varphi^*(y)\,\mathrm{d}y}{\int_M \varphi^*(y)\,\mathrm{d}y} & \text{if } P \text{ is positive-critical in } M, \\ 1 & \text{otherwise.} \end{cases}$$

Suppose further that P is not positive-critical in M, and f is a bounded continuous function such that $\liminf_{x\to\infty} f(x) = \varepsilon > 0$. Then

$$\liminf_{t\to\infty} \int_M k_P^M(x,y,t) f(y)\,\mathrm{d}y \geq \varepsilon. \tag{6.2}$$

Hence, if the integrability condition of Corollary 6.2 is not satisfied, then the large time behavior of the minimal solution of the Cauchy problem may be complicated. The following example of W. Kirsch and B. Simon [34] demonstrates this phenomenon.

Example 6.3. Consider the heat equation in $\mathbb{R}^d$. Let $R_j := \mathrm{e}^{\mathrm{e}^j}$ and let

$$f(x) := 2 + (-1)^j \qquad \text{if} \quad R_j < \sup_{1\leq i\leq d} |x_i| < R_{j+1},\ j \geq 1.$$

Let u be the minimal solution of the Cauchy problem with initial data f. Then for $t \sim R_j R_{j+1}$ one has that $u(0,t) \sim 2 + (-1)^j$, and thus $u(0,t)$ does not have a limit. Note that by Lemma 4.1, for $d = 1$, $u(x,t)$ has exactly the same asymptotic behavior as $u(0,t)$ for all $x \in \mathbb{R}$.

In fact, it was proved in [56] that for the heat equation on $\mathbb{R}^d$, the following holds: for any bounded function f defined on $\mathbb{R}^d$, the limit

$$\lim_{t\to\infty} \int_{\mathbb{R}^d} k_{-\Delta}^{\mathbb{R}^d}(x,y,t) f(y)\,\mathrm{d}y$$

exists, if and only if the limit

$$\lim_{R\to\infty} \frac{1}{|B(x,R)|} \int_{B(x,R)} f(y)\,\mathrm{d}y$$

exists. Moreover, the values of the two limits are equal. For an extension of the above result see [31]. We note that such a theorem is false if the average value of f is taken on solid cubes.

The next three corollaries concern elliptic operators on manifolds.

Corollary 6.4 ([12]). *Let M be a noncompact complete Riemannian manifold, and denote by Δ the corresponding Laplace–Beltrami operator. Then*

$$\ell_0 := \lim_{t\to\infty} k^M_{-\Delta}(x,y,t) = 0 \tag{6.3}$$

if and only if M has an infinite volume.

Proof. If M has a finite volume, then $-\Delta$ is positive-critical in M, and by Theorem 1.3, we have $\ell_0 = \big(\mathrm{vol}(M)\big)^{-1} > 0$.

Suppose now that M has an infinite volume. If $\lambda_0 > 0$, Corollary 6.1 implies that $\ell_0 = 0$. On the other hand, if $\lambda_0 = 0$, then since $u = \mathbf{1}$ is a positive harmonic function which is not in $L^2(M)$, the uniqueness of the ground state implies that $-\Delta$ is not positive-critical in M. Hence, by Theorem 1.3 we have $\ell_0 = 0$. □

Before studying the next two results we recall three basic notions from the theory of manifolds with group actions.

Definition 6.5. Let G be a group, and suppose that G acts on M. For any real continuous function v and $g \in G$, denote by v^g the function defined by $v^g(x) := v(gx)$. Let $\mathbb{R}^* = \mathbb{R} \setminus \{0\}$ be the real multiplicative group.

1. A nonzero real continuous function f on M is called *G-multiplicative* if there exists a group homomorphism $\gamma : G \to \mathbb{R}^*$, such that
$$f(gx) = \gamma(g) f(x) \qquad \forall g \in G, x \in M.$$
2. A G-group action on M is *compactly generating* if there exists $K \Subset M$ such that $GK = M$ (see [38]).
3. The operator P is said to be G-equivariant if
$$P[u^g] = (P[u])^g \qquad \forall g \in G.$$

Corollary 6.6 (cf. [12]). *Suppose that a noncompact manifold M is a covering of a compact Riemannian manifold, and consider the Laplace–Beltrami operator Δ on M. Then*

$$\ell := \lim_{t\to\infty} \mathrm{e}^{\lambda_0 t} k^M_{-\Delta}(x,y,t) = 0. \tag{6.4}$$

In particular, $-\Delta - \lambda_0$ is not positive-critical in M.

Proof. Suppose that $\ell > 0$. By Theorem 1.3, the operator $-\Delta - \lambda_0$ is positive-critical in M, and in particular, the ground state φ is in $L^2(M)$. The uniqueness of the ground state implies that φ is G-multiplicative, where G is the deck transformation. But this contradicts the assumption that $\varphi \in L^2$, since G is an infinite group. □

The following corollary deals with manifolds with group actions and *general* equivariant operators, without any assumption on the growth of the acting groups. It generalizes Corollary 6.6, and seems to be new.

Corollary 6.7. *Let M be a noncompact manifold, and let G be a group. Suppose that G acts on M, and that the G-group action on M is compactly generating. Assume that P is a G-equivariant second-order elliptic operator of the form* (2.1) *which is defined on M. Suppose further that any nonzero G-multiplicative $C^{2,\alpha}$-function is not integrable on M. Then*

$$\ell := \lim_{t\to\infty} \mathrm{e}^{\lambda_0 t} k_P^M(x,y,t) = 0. \tag{6.5}$$

Proof. Suppose that $\ell > 0$. By Theorem 1.3, the operator $P-\lambda_0$ is positive-critical in M. In particular, $\dim \mathcal{C}_{P-\lambda_0}(M) = \dim \mathcal{C}_{P^*-\lambda_0}(M) = 1$. By the uniqueness of the ground state, it follows that the corresponding ground states φ and φ^* are G-multiplicative. Therefore, their product $\varphi\varphi^*$ is also G-multiplicative, and we arrived at a contradiction since by our assumption a nonzero G-multiplicative $C^{2,\alpha}$-function is not integrable on M. □

Remark 6.8.

1. Corollary 6.7 clearly applies to the case where M is a regular covering of a compact Riemannian manifold, and G is the corresponding deck transformation. In fact, in the critical case, by [38, Theorem 5.17], the product of the ground states is a positive G-invariant function, and therefore it is not integrable on M.
2. Corollary 6.7 applies in particular to the case where P is defined on $\mathbb{R}^d$, and P is $\mathbb{Z}^d$-equivariant (that is, P has $\mathbb{Z}^d$-periodic coefficients). In this case it is known that $P-\lambda_0$ is (null)-critical if and only if $d = 1, 2$. For further related results, see [38].

Finally, let us introduce an important subclass of elliptic operators P such that $P-\lambda_0$ is positive-critical in M.

Definition 6.9. Assume that P is symmetric and $P-\lambda_0$ is positive-critical in M with a ground state φ satisfying the normalization condition $\|\varphi\|_{L^2(M)} = 1$. Let $T_P^M(t)$ be the corresponding (Dirichlet) semigroup on $L^2(M)$ generated by P. We say that $T_P^M(t)$ is *intrinsically ultracontractive* if for any $t > 0$ there exists a positive-constant C_t such that

$$0 \leq \mathrm{e}^{\lambda_0 t} k_P^M(x,y,t) \leq c_t \varphi(x)\varphi(y) \qquad \forall x, y \in M.$$

Example 6.10. If M is a smooth bounded domain and $P := -\Delta$, then the semigroup $T_P^M(t)$ is intrinsically ultracontractive on $L^2(M)$. Also, let $M := \mathbb{R}^d$ and $P := -\Delta + (1+|x|^2)^{\alpha/2}$, where $\alpha \in \mathbb{R}$. Then $T_P^M(t)$ is intrinsically ultracontractive on $L^2(M)$ if and only if $\alpha > 2$ (see also [20, 44] and references therein).

It turns out that in the intrinsically ultracontractive case the rate of the convergence (as $t \to \infty$) of the h-transformed heat kernel is uniformly exponentially fast.

Theorem 6.11 ([20, Theorem 4.2.5]). *Assume that P is symmetric and subcritical in M, and suppose that $T_P^M(t)$ is intrinsically ultracontractive on $L^2(M)$. Then* *there exists a complete orthonormal set* $\{\varphi_j\}_{j=0}^{\infty}$ *in* $L^2(M)$ *such that* $\varphi_0 = \varphi$*, and for any* $j \geq 0$ *the function* φ_j *is an eigenfunction of the Friedrichs extension of the operator* P *with eigenvalue* λ_j*, where* $\{\lambda_j\}$ *is nondecreasing. Moreover, the heat kernel has the eigenfunction expansion* (2.9)*, and there exist positive-constants* C *and* δ *such that*

$$\left| \mathrm{e}^{\lambda_0 t} \frac{k_P^M(x,y,t)}{\varphi_0(x)\varphi_0(y)} - 1 \right| \leq C\mathrm{e}^{-\delta t} \qquad \forall x, y \in M, t > 1.$$

Furthermore, for any $\varepsilon > 0$ *the series*

$$\frac{k_P^M(x,y,t)}{\varphi_0(x)\varphi_0(y)} = \sum_{n=0}^{\infty} \mathrm{e}^{-\lambda_n t} \frac{\varphi_n(x)\varphi_n(y)}{\varphi_0(x)\varphi_0(y)}$$

converges uniformly on $M \times M \times [\varepsilon, \infty)$*.*

Remark 6.12. Murata [45] proved that if $T_P^M(t)$ is intrinsically ultracontractive on $L^2(M)$, then $\mathbf{1}$ is a small perturbation of P in M. In particular, for any $n \geq 0$ the function φ_n/φ_0 is bounded, and has a continuous extension up to the Martin boundary of M (with respect to P) [50]. On the other hand, an example of Bañuelos and Davis in [7] gives us a finite area domain $M \subset \mathbb{R}^2$ such that $\mathbf{1}$ is a small perturbation of the Laplacian in M, but the corresponding semigroup is not intrinsically ultracontractive.

Remark 6.13. In the null-recurrent case, the heat kernel may decay very slowly as $t \to \infty$, and one can construct a complete Riemannian manifold M such that all its Riemannian products $M^j, j \geq 1$ are null-recurrent with respect to the Laplace–Beltrami operator on M^j (see [19]).

7. Davies' conjecture concerning strong ratio limit

Having proved in Section 5 that $\lim_{t\to\infty} \mathrm{e}^{\lambda_0 t} k_P^M(x,y,t)$ always exists, we next ask how fast this limit is approached. It is natural to conjecture that the limit is approached equally fast for different points $x, y \in M$. Note that in the context of Markov chains, such an (*individual*) *strong ratio limit property* is in general not true [13]. The following conjecture was raised by E. B. Davies [22] in the selfadjoint case.

Conjecture 7.1 (Davies' conjecture). *Let* $Lu = u_t + P(x, \partial_x)u$ *be a parabolic operator which is defined on a noncompact Riemannian manifold* M*, and assume that* $\lambda_0(P, M) \geq 0$*. Fix a reference point* $x_0 \in M$*. Then*

$$\lim_{t\to\infty} \frac{k_P^M(x,y,t)}{k_P^M(x_0,x_0,t)} = a(x,y) \tag{7.1}$$

exists and is positive for all $x, y \in M$*.*

The aim of the present section is to discuss Conjecture 7.1 and closely related problems, and to obtain some results under minimal assumptions. Since, the conjecture does not depend on the value of λ_0, we assume throughout the present section that $\lambda_0 = 0$.

Conjecture 7.1 was recently disproved by G. Kozma [35] in the *discrete* setting:

Theorem 7.2 (Kozma [35]). *There exists a connected graph G with bounded weights and two vertices $x, y \in G$ such that*

$$\lim_{n\to\infty} \frac{k(x,x,n)}{k(y,y,n)} \tag{7.2}$$

does not exist, where k is the heat kernel of the lazy random walk such that the walker, at every step, chooses with probability $1/2$ to stay in place, and with probability $1/2$ to move to one of the neighbors (with probability proportional to the given weights).

In addition, Kozma indicates in [35] how the construction might be carried out in the category of Laplace–Beltrami operators on manifolds with bounded geometry. As noted in [35], the bounded weights property in the graph's setting is the analogue to the bounded geometry property in the manifold setting, a property that in fact was not assumed in Davies' conjecture. We note that in Kozma's example the ratio $\frac{k(x,x,n)}{k(y,y,n)}$ is bounded between two constants that are independent of t.

Nevertheless, as we show below, there are many situations where Conjecture 7.1 holds true.

Remark 7.3.

1. Theorem 1.3 implies that Conjecture 7.1 holds true in the positive-critical case, therefore, we assume throughout the present section that P *is not positive-critical.*
2. We also note that if P is *symmetric*, then the conjecture holds if
$$\dim \mathcal{C}_{P-\lambda_0}(M) = 1, \tag{7.3}$$
(i.e., in the "Liouvillian" case) see [4, Corollary 2.7]. In particular, it holds true for *critical selfadjoint* operators. It also holds for the Laplace–Beltrami operator on a complete Riemannian manifold of dimension d with nonnegative Ricci curvature [22].
3. Recently Agmon [2] obtained the exact asymptotics (in (x, y, t)) of the heat kernel for a $\mathbb{Z}^d$-periodic (non-selfadjoint) operator P on $\mathbb{R}^d$, and for an equivariant operator P defined on *abelian* cocompact covering manifold M. In particular, it follows from Agmon's results that Conjecture 7.1 holds true in these cases. Note that in these cases (and even in the case of *nilpotent* cocompact covering) it is known [38] that
$$\dim \mathcal{C}_{P-\lambda_0}(M) = \dim \mathcal{C}_{P^*-\lambda_0}(M) = 1. \tag{7.4}$$
4. For other particular cases where the conjecture holds true see [4, 10, 14, 15, 22, 65].

Remark 7.4. It would be interesting to prove Conjecture 7.1 at least under the assumption

$$\dim \mathcal{C}_{P-\lambda_0}(M) = \dim \mathcal{C}_{P^*-\lambda_0}(M) = 1, \tag{7.5}$$

which holds true in the critical case and in many important subcritical (Liouvillian) cases. For a probabilistic interpretation of Conjecture 7.1, see [4].

Remark 7.5. Let $t_n \to \infty$. By a standard parabolic argument, we may extract a subsequence $\{t_{n_k}\}$ such that for every $x, y \in M$ and $s < 0$

$$a(x, y, s) := \lim_{k\to\infty} \frac{k_P^M(x, y, s + t_{n_k})}{k_P^M(x_0, y_0, t_{n_k})} \tag{7.6}$$

exists. Moreover, $a(\cdot, y, \cdot) \in \mathcal{H}_P(M \times \mathbb{R}_-)$, and $a(x, \cdot, \cdot) \in \mathcal{H}_{P^*}(M \times \mathbb{R}_-)$. Note that in the selfadjoint case, we can extract a subsequence $\{t_{n_k}\}$ such that the limit function a satisfies $a(\cdot, y, \cdot) \in \mathcal{H}_P(M \times \mathbb{R})$ [52].

Remark 7.6. Consider the complete two-dimensional Riemannian manifold M that is constructed in [49]. Then M does not admit nonconstant positive harmonic functions, $\lambda_0(-\Delta, M) = 0$. Nevertheless, the heat operator does not admit any λ_0-invariant positive solution. In particular, M is stochastically incomplete (this construction disproves Stroock's conjecture concerning the existence of a λ_0-invariant positive solution).

On the other hand, since M is Liouvillian, Remark 7.3 implies that Conjecture 7.1 holds true on M. Hence, the limit function

$$a(x, y) := \lim_{t\to\infty} \frac{k_{-\Delta}^M(x, y, t)}{k_{-\Delta}^M(x_0, x_0, t)} \tag{7.7}$$

(which equals to the constant function $\mathbf{1}$) is not a λ_0-invariant positive solution. Compare this with [22, Theorem 25] and the discussion therein above Lemma 26. In particular, it follows that the function

$$\mu(x) := \sup \left\{ \sqrt{\frac{K_P^M(x, x, t)}{K_P^M(x_0, x_0, t)}} \;\Big|\; 1 \le t < \infty \right\}$$

is not slowly increasing at infinity in the sense of [22].

Suppose that P is symmetric (and $\lambda_o = 0$). Using (2.9) and a standard exhaustion argument, it follows [22] that for a fixed $x \in M$, the function $t \mapsto k_P^M(x, x, t)$ is a nonincreasing log-convex function, and therefore, a polarization argument implies that the following strong ratio property holds true.

$$\lim_{t\to\infty} \frac{k_P^M(x, y, t + s)}{k_P^M(x, y, t)} = 1 \qquad \forall x, y \in M,\ s \in \mathbb{R}. \tag{7.8}$$

In the nonsymmetric case, Corollary 6.1 and the parabolic Harnack inequality imply:

Lemma 7.7 ([52]). *For every $x, y \in M$ and $s \in \mathbb{R}$, we have that*

$$\liminf_{t\to\infty} \frac{k_P^M(x,y,t+s)}{k_P^M(x,y,t)} \leq 1 \leq \limsup_{t\to\infty} \frac{k_P^M(x,y,t+s)}{k_P^M(x,y,t)} . \tag{7.9}$$

In particular, if $\lim_{t\to\infty}[k_P^M(x,y,t+s)/k_P^M(x,y,t)]$ *exists, it equals to* 1.

Remark 7.8. If there exist $x_0, y_0 \in M$ and $0 < s_0 < 1$ such that

$$M(x_0,y_0,s_0) := \limsup_{t\to\infty} \frac{k_P^M(x_0,y_0,t+s_0)}{k_P^M(x_0,y_0,t)} < \infty, \tag{7.10}$$

then by the parabolic Harnack inequality, for all $x, y, z, w \in K \subset\subset M$, $t > 1$, we have the following Harnack inequality of elliptic type:

$$k_P^M(z,w,t) \leq C_1 k_P^M(x_0,y_0,t+\frac{s_0}{2}) \leq C_2 k_P^M(x_0,y_0,t-\frac{s_0}{2}) \leq C_3 k_P^M(x,y,t). \tag{7.11}$$

Similarly, (7.10) implies that for all $x, y \in M$ and $r \in \mathbb{R}$:

$$\begin{aligned} 0 < m(x,y,r) &:= \liminf_{t\to\infty} \frac{k_P^M(x,y,t+r)}{k_P^M(x_0,y_0,t)} \\ &\leq \limsup_{t\to\infty} \frac{k_P^M(x,y,t+r)}{k_P^M(x_0,y_0,t)} = M(x,y,r) < \infty. \end{aligned}$$

Note that (7.10) is obviously satisfied in the symmetric case, and consequently (7.11) holds true [20, Theorem 10].

It turns out that the validity of the strong limit property (7.8) (in the non-symmetric case) implies the validity of Davies' conjecture if in addition (7.5) is satisfied. We have:

Lemma 7.9 ([52]).

(a) *The following assertions are equivalent:*

(i) *For each $x, y \in M$ there exists a sequence $s_j \to 0$ of negative numbers such that for all $j \geq 1$, and $s = s_j$, we have*

$$\lim_{t\to\infty} \frac{k_P^M(x,y,t+s)}{k_P^M(x,y,t)} = 1. \tag{7.12}$$

(ii) *The ratio limit in* (7.12) *exists for any $x, y \in M$ and $s \in \mathbb{R}$.*

(iii) *Any limit function $u(x,y,s)$ of the quotients $\frac{k_P^M(x,y,t_n+s)}{k_P^M(x_0,x_0,t_n)}$ with $t_n \to \infty$ does not depend on s and has the form $u(x,y)$, where $u(\cdot,y) \in \mathcal{C}_P(M)$ for every $y \in M$ and $u(x,\cdot) \in \mathcal{C}_{P^*}(M)$ for every $x \in M$.*

(b) *If one assumes further that* (7.5) *is satisfied, then Conjecture* 7.1 *holds true. Moreover, Conjecture* 7.1 *holds true if $M \subsetneqq \mathbb{R}^d$ is a smooth unbounded domain, P and P^* are (up to the boundary) smooth operators,* (7.12) *holds true, and*

$$\dim \mathcal{C}_P^0(M) = \dim \mathcal{C}_{P^*}^0(M) = 1, \tag{7.13}$$

where $\mathcal{C}_P^0(M)$ denotes the cone of all functions in $\mathcal{C}_P(M)$ that vanish on ∂M.

Proof. (a) By Lemma 7.7, if the limit in (7.12) exists, then it is 1.

(i) ⇒ (ii). Fix $x_0, y_0 \in M$, and take $s_0 < 0$ for which the limit (7.12) exists. It follows that any limit solution $u(x, y, s) \in \mathcal{H}_P(M \times \mathbb{R}_-)$ of a sequence $\left\{\frac{k_P^M(x,y,t_n+s)}{k_P^M(x_0,y_0,t_n)}\right\}$ with $t_n \to \infty$ satisfies $u(x_0, y_0, s + s_0) = u(x_0, y_0, s)$ for all $s < 0$. So, $u(x_0, y_0, \cdot)$ is s_0-periodic. It follow from our assumption and the continuity of u that $u(x_0, y_0, \cdot)$ is the constant function. Since this holds for all $x, y \in M$ and u, it follows that (7.12) holds for any $x, y \in M$ and $s \in \mathbb{R}$.

(ii) ⇒ (iii). Fix $y \in M$. By Remark 7.5, any limit function u of the sequence $\left\{\frac{k_P^M(x,y,t_n+s)}{k_P^M(x_0,x_0,t_n)}\right\}$ with $t_n \to \infty$ belongs to $\mathcal{H}_P(M \times \mathbb{R}_-)$. Since

$$\frac{k_P^M(x,y,t+s)}{k_P^M(x_0,x_0,t)} = \frac{k_P^M(x,y,t)}{k_P^M(x_0,x_0,t)}\,\frac{k_P^M(x,y,t+s)}{k_P^M(x,y,t)}\,, \tag{7.14}$$

(7.12) implies that such a u does not depend on s. Therefore, $u = u(x, y)$, where $u(\cdot, y) \in \mathcal{C}_P(M)$ and $u(x, \cdot) \in \mathcal{C}_{P^*}(M)$.

(iii) ⇒ (i). Write

$$\frac{k_P^M(x,y,t+s)}{k_P^M(x,y,t)} = \frac{k_P^M(x,y,t+s)}{k_P^M(x_0,x_0,t)}\,\frac{k_P^M(x_0,x_0,t)}{k_P^M(x,y,t)}\,. \tag{7.15}$$

Let $t_n \to \infty$ be a sequence such that the sequence $\left\{\frac{k_P^M(x,y,t_n+s)}{k_P^M(x_0,x_0,t_n)}\right\}$ converges to a solution in $\mathcal{H}_P(M \times \mathbb{R}_-)$. By our assumption, we have

$$\lim_{n\to\infty} \frac{k_P^M(x,y,t_n+s)}{k_P^M(x_0,x_0,t_n)} = \lim_{n\to\infty} \frac{k_P^M(x,y,t_n)}{k_P^M(x_0,x_0,t_n)} = u(x,y) > 0,$$

which together with (7.15) implies (7.12) for all $s \in \mathbb{R}$.

(b) The uniqueness and (iii) imply that $\frac{k_P^M(x,y,t+s)}{k_P^M(x_0,x_0,t)} \to \frac{u(x)u^*(y)}{u(x_0)u^*(x_0)}$, where $u \in \mathcal{C}_P(M)$ and $u^* \in \mathcal{C}_{P^*}(M)$, and Conjecture 7.1 holds. □

Remark 7.10. Assume that one of the assumptions of part (a) of Lemma 7.9 is satisfied. Then by the lemma, any limit function of the sequence $\left\{\frac{k_P^M(x,y,t_n+s)}{k_P^M(x_0,x_0,t_n)}\right\}$ is of the form $a(x, y)$, where for every $y \in M$, the function $a(\cdot, y) \in \mathcal{C}_P(M)$, and $a(x, \cdot) \in \mathcal{C}_{P^*}(M)$ for every $x \in M$. But in general, $a(x, y)$ does not need to be a *product* of solutions of the equations $Pu = 0$ and $P^*u = 0$, as is demonstrated in [15], in the hyperbolic space, and in [52, Example 4.2].

In the null-critical case we have:

Lemma 7.11 ([52]). *Suppose that P is null-critical, and for each $x, y \in M$ there exists a sequence $\{s_j\}$ of negative numbers such that $s_j \to 0$, and*

$$\liminf_{t\to\infty} \frac{k_P^M(x,y,t+s)}{k_P^M(x,y,t)} \geq 1 \tag{7.16}$$

for $s = s_j$, $j = 1, 2, \ldots$. Then Conjecture 7.1 holds true.

Proof. Let $u(x,y,s)$ be a limit function of a sequence $\left\{\frac{k_P^{\mathcal{M}}(x,y,t_n+s)}{k_P^{\mathcal{M}}(x_0,x_0,t_n)}\right\}$ with $t_n \to \infty$ and $s<0$. By our assumption, $u(x,y,s+s_j) \geq u(x,y,s)$, and therefore, $u_s(x,y,s) \leq 0$ for all $s<0$. Thus, $u(\cdot,y,s)$ (respect., $u(x,\cdot,s)$) is a positive supersolution of the equation $Pu=0$ (respect., $P^*u=0$) in $\mathcal{M}$. Since P is critical, it follows that $u(\cdot,y,s) \in \mathcal{C}_P(\mathcal{M})$ (respect., $u(x,\cdot,s) \in \mathcal{C}_{P^*}(\mathcal{M})$), and hence $u_s(x,y,s)=0$. By the uniqueness, u equals to $\frac{\varphi(x)\varphi^*(y)}{\varphi(x_0)\varphi^*(x_0)}$, and Conjecture 7.1 holds true. □

The large time behavior of quotients of the heat kernel is obviously closely related to the parabolic Martin boundary (for the parabolic Martin boundary theory see [16, 23, 45]). The next result relates Conjecture 7.1 and the parabolic Martin compactification of $\mathcal{H}_P(M \times \mathbb{R}_-)$.

Theorem 7.12 ([52]). *Assume that* (7.10) *holds true for some* $x_0, y_0 \in M$, *and* $s_0>0$. *Then the following assertions are equivalent:*

(i) *Conjecture* 7.1 *holds true for a fixed* $x_0 \in M$.

(ii)
$$\lim_{t\to\infty} \frac{k_P^M(x,y,t)}{k_P^M(x_1,y_1,t)} \tag{7.17}$$
exists, and the limit is positive for every $x,y,x_1,y_1 \in M$.

(iii)
$$\lim_{t\to\infty} \frac{k_P^M(x,y,t)}{k_P^M(y,y,t)}, \quad \text{and} \quad \lim_{t\to\infty} \frac{k_P^M(x,y,t)}{k_P^M(x,x,t)} \tag{7.18}$$
exist, and these ratio limits are positive for every $x,y \in M$.

(iv) *For any* $y \in M$ *there is a unique nonzero parabolic Martin boundary point* $\bar{y}$ *for the equation* $Lu=0$ *in* $M\times\mathbb{R}$ *which corresponds to any sequence of the form* $\{(y,-t_n)\}_{n=1}^\infty$ *such that* $t_n \to \infty$, *and for any* $x \in M$ *there is a unique nonzero parabolic Martin boundary point* $\bar{x}$ *for the equation* $u_t+P^*u=0$ *in* $M\times\mathbb{R}$ *which corresponds to any sequence of the form* $\{(x,-t_n)\}_{n=1}^\infty$ *such that* $t_n\to\infty$.

Moreover, if Conjecture 7.1 *holds true, then for any fixed* $y\in M$ *(respect.,* $x \in M$*), the limit function* $a(\cdot,y)$ *(respect.,* $a(x,\cdot)$*) is a positive solution of the equation* $Pu=0$ *(respect.,* $P^*u=0$*). Furthermore, the Martin functions of part* (iv) *are time independent, and* (7.12) *holds for all* $x,y\in M$ *and* $s \in \mathbb{R}$.

Proof. (i) ⇒ (ii) follows from the identity
$$\frac{k_P^M(x,y,t)}{k_P^M(x_1,y_1,t)} = \frac{k_P^M(x,y,t)}{k_P^M(x_0,x_0,t)} \cdot \left(\frac{k_P^M(x_1,y_1,t)}{k_P^M(x_0,x_0,t)}\right)^{-1}.$$

(ii) ⇒ (iii). Take $x_1=y_1=y$ and $x_1=y_1=x$, respectively.

(iii) ⇒ (iv). It is well known that the Martin compactification does not depend on the fixed reference point x_0. So, fix $y\in M$ and take it also as a reference point. Let $\{-t_n\}$ be a sequence such that $t_n\to\infty$ and such that the Martin sequence

$\left\{\frac{k_P^M(x,y,t+t_n)}{k_P^M(y,y,t_n)}\right\}$ converges to a Martin function $K_P^M(x,\bar{y},t)$. By our assumption, for any t we have

$$\lim_{n\to\infty}\frac{k_P^M(x,y,t+t_n)}{k_P^M(y,y,t+t_n)}=\lim_{\tau\to\infty}\frac{k_P^M(x,y,\tau)}{k_P^M(y,y,\tau)}=b(x)>0,$$

where b does not depend on the sequence $\{-t_n\}$. On the other hand,

$$\lim_{n\to\infty}\frac{k_P^M(y,y,t+t_n)}{k_P^M(y,y,t_n)}=K_P^M(y,\bar{y},t)=f(t).$$

Since

$$\frac{k_P^M(x,y,t+t_n)}{k_P^M(y,y,t_n)}=\frac{k_P^M(x,y,t+t_n)}{k_P^M(y,y,t+t_n)}\cdot\frac{k_P^M(y,y,t+t_n)}{k_P^M(y,y,t_n)},$$

we have

$$K_P^M(x,\bar{y},t)=b(x)f(t).$$

By separation of variables, there exists a constant λ such that

$$Pb-\lambda b=0 \quad \text{on } M, \qquad f'+\lambda f=0 \quad \text{on } \mathbb{R},\ \ f(0)=1.$$

Since b does not depend on the sequence $\{-t_n\}$, it follows in particular, that λ does not depend on this sequence. Thus, $\lim_{\tau\to\infty}\frac{k_P^M(y,y,t+\tau)}{k_P^M(y,y,\tau)}=f(t)=\mathrm{e}^{-\lambda t}$. Lemma 7.7 implies that $\lambda=0$. It follows that b is a positive solution of the equation $Pu=0$, and

$$K_P^M(x,\bar{y},t)=\lim_{\tau\to-\infty}\frac{k_P^M(x,y,t-\tau)}{k_P^M(y,y,-\tau)}=b(x). \tag{7.19}$$

The dual assertion can be proved similarly.

(iv) $\Rightarrow$ (i). Let $K_P^M(x,\bar{y},t)$ be the Martin function given in (iv), and $s_0>0$ such that $K_P^M(x_0,\bar{y},s_0/2)>0$. Consequently, $K_P^M(x,\bar{y},s)>0$ for $s\geq s_0$. Using the substitution $\tau=s+s_0$ we obtain

$$\begin{aligned}\lim_{\tau\to\infty}\frac{k_P^M(x,y,\tau)}{k_P^M(x_0,x_0,\tau)}&=\lim_{s\to\infty}\left\{\frac{k_P^M(x,y,s+s_0)}{k_P^M(y,y,s)}\frac{k_P^M(y,y,s)}{k_P^M(x_0,y,s+2s_0)}\frac{k_P^M(x_0,y,s+2s_0)}{k_P^M(x_0,x_0,s+s_0)}\right\}\\&=\frac{K_P^M(x,\bar{y},s_0)K_{P^*}^M(\overline{x_0},y,s_0)}{K_P^M(x_0,\bar{y},2s_0)}.\end{aligned}$$

The last assertion of the theorem follows from (7.19) and Lemma 7.9. □

Finally we mention a problem which was raised by Burdzy and Salisbury [9] for $P=-\Delta$ and $\mathcal{M}\subset\mathbb{R}^d$.

Question 7.13 ([52]). *Assume that* $\lambda_0=0$. *Determine which minimal functions (in the sense of Martin's boundary) in* $\mathcal{C}_P(\mathcal{M})$ *are minimal in* $\mathcal{H}_P(\mathcal{M}\times\mathbb{R}_-)$. *In particular, is it true that in the critical case, the ground state* φ *is minimal in* $\mathcal{H}_P(\mathcal{M}\times\mathbb{R}_-)$*?*

8. Comparing decay of critical and subcritical heat kernels

In this section we are concerned with the large time behavior of the heat kernel k_P^M with regards to the criticality versus subcriticality property of the operator P. Since for any fixed $x, y \in M$, $x \neq y$, we have that $k_P^M(x,y,\cdot) \in L^1(\mathbb{R}_+)$ if and only if P is subcritical, it is natural to conjecture that *under some assumptions* the heat kernel of a subcritical operator P_+ in M decays (in time) faster than the heat kernel of a critical operator P_0 in M. Hence, our aim is to discuss the following conjecture in *general* settings.

Conjecture 8.1 ([24]). *Let P_+ and P_0 be respectively subcritical and critical operators in M. Then*

$$\lim_{t\to\infty} \frac{k_{P_+}^M(x,y,t)}{k_{P_0}^M(x,y,t)} = 0 \tag{8.1}$$

locally uniformly in $M \times M$.

Conjecture 8.1 was stimulated by the following conjecture of D. Krejčiřík and E. Zuazua [36]:

Let P_+ and P_0 be, respectively, selfadjoint *subcritical and critical operators defined on $L^2(M, \mathrm{d}x)$. Then*

$$\lim_{t\to\infty} \frac{\|\mathrm{e}^{-P_+ t}\|_{L^2(M, W\,\mathrm{d}x)\to L^2(M,\mathrm{d}x)}}{\|\mathrm{e}^{-P_0 t}\|_{L^2(M, W\,\mathrm{d}x)\to L^2(M,\mathrm{d}x)}} = 0 \tag{8.2}$$

for some positive weight function W.

Remark 8.2. Theorem 1.3 implies that Conjecture 8.1 obviously holds true if P_0 is positive-critical. Moreover, by Corollary 6.1 the conjecture also holds true if $\lambda_0(P_+, M) > 0$. Therefore, throughout this section we assume that $\lambda_0(P_+, M) = 0$, and P_0 is null-critical in M.

Example 8.3. In [41] M. Murata obtained the exact asymptotic for the heat kernels of nonnegative Schrödinger operators with *short-range* (real) potentials defined on $\mathbb{R}^d$, $d \geq 1$. In particular, [41, Theorems 4.2 and 4.4] imply that Conjecture 8.1 holds true for such operators.

The following theorem deals with the *symmetric* case.

Theorem 8.4 ([24]). *Let the subcritical operator P_+ and the critical operator P_0 be symmetric in M of the form*

$$Pu = -m^{-1}\mathrm{div}(mA\nabla u) + Vu. \tag{8.3}$$

Assume that A_+ and A_0, the sections on M of $\mathrm{End}(TM)$, *and the weights m_+ and m_0, corresponding to P_+ and P_0, respectively, satisfy the following matrix inequality*

$$m_+(x)A_+(x) \leq Cm_0(x)A_0(x) \qquad \text{for a.e. } x \in M, \tag{8.4}$$

where C is a positive constant. Assume further that for some fixed $y_1 \in M$ there exists a positive constant C satisfying the following condition: for each $x \in M$ there exists $T(x) > 0$ such that

$$k_{P_+}^M(x, y_1, t) \leq C k_{P_0}^M(x, y_1, t) \qquad \forall t > T(x). \tag{8.5}$$

Then

$$\lim_{t\to\infty} \frac{k_{P_+}^M(x, y, t)}{k_{P_0}^M(x, y, t)} = 0 \tag{8.6}$$

locally uniformly in $M \times M$.

Proof. Recall that in light of Remark 8.2 we assume that $\lambda_0(P_+, M) = 0$. Suppose to the contrary that for some $x_0, y_0 \in M$ there exists a sequence $\{t_n\}$ such that $t_n \to \infty$, and

$$\lim_{n\to\infty} \frac{k_{P_+}^M(x_0, y_0, t_n)}{k_{P_0}^M(x_0, y_0, t_n)} = K > 0. \tag{8.7}$$

Consider the sequence of functions $\{u_n\}_{n=1}^{\infty}$ defined by

$$u_n(x, s) := \frac{k_{P_+}^M(x, y_0, t_n + s)}{k_{P_0}^M(x_0, y_0, t_n)} \qquad x \in M, \; s \in \mathbb{R}.$$

We note that

$$u_n(x, s) = \frac{k_{P_+}^M(x, y_0, t_n + s)}{k_{P_+}^M(x_0, y_0, t_n)} \times \frac{k_{P_+}^M(x_0, y_0, t_n)}{k_{P_0}^M(x_0, y_0, t_n)} .$$

Therefore, by assumption (8.7) and Remark 7.5 it follows that we may subtract a subsequence which we rename by $\{u_n\}$ such that

$$\lim_{n\to\infty} u_n(x, s) = u_+(x, s),$$

where $u_+ \in \mathcal{H}_{P_+}(M \times \mathbb{R})$ and $u_+ \gneqq 0$.

On the other hand,

$$v_n(x) := \frac{k_{P_+}^M(x, y_0, t_n)}{k_{P_0}^M(x_0, y_0, t_n)} = u_n(x, s) \frac{k_{P_+}^M(x, y_0, t_n)}{k_{P_+}^M(x, y_0, t_n + s)} .$$

By our assumption, $\lambda_0(P_+, M) = 0$ and P_+ is symmetric, therefore (7.8) implies that

$$\lim_{n\to\infty} \frac{k_{P_+}^M(x, y_0, t_n)}{k_{P_+}^M(x, y_0, t_n + s)} = 1.$$

Therefore,

$$\lim_{n\to\infty} v_n(x) = \lim_{n\to\infty} u_n(x, s) = u_+(x, s),$$

and u_+ does not depend on s, and hence u_+ is a positive solution of the elliptic equation $P_+ u = 0$ in M and we have

$$\lim_{n\to\infty} \frac{k_{P_+}^M(x, y_0, t_n)}{k_{P_0}^M(x_0, y_0, t_n)} = u_+(x). \tag{8.8}$$

On the other hand, by Remark 7.3 we have

$$\lim_{n\to\infty}\frac{k^M_{P_0}(x,y_0,t_n)}{k^M_{P_0}(x_0,y_0,t_n)}=\frac{\varphi(x)}{\varphi(x_0)}=:u_0(x), \tag{8.9}$$

where φ is the ground state of P_0.

Combining (8.8) and (8.9), we obtain

$$\lim_{n\to\infty}\frac{k^M_{P_+}(x,y_0,t_n)}{k^M_{P_0}(x,y_0,t_n)}=\lim_{n\to\infty}\left\{\frac{\frac{k^M_{P_+}(x,y_0,t_n)}{k^M_{P_0}(x_0,y_0,t_n)}}{\frac{k^M_{P_0}(x,y_0,t_n)}{k^M_{P_0}(x_0,y_0,t_n)}}\right\}=\frac{u_+(x)}{u_0(x)}. \tag{8.10}$$

On the other hand, by assumption (8.5) and the parabolic Harnack inequality there exists a positive constant C_1 which depends on P_+, P_0, y_0, y_1 such that

$$\begin{aligned}C_1^{-1}k^M_{P_+}(x,y_0,t-1)&\le k^M_{P_+}(x,y_1,t)\\ &\le Ck^M_{P_0}(x,y_1,t)\le CC_1k^M_{P_0}(x,y_0,t+1)\quad \forall x\in M, t>T(x).\end{aligned} \tag{8.11}$$

Moreover, by (7.8) we have

$$\lim_{t\to\infty}\frac{k^M_{P_+}(x,y_0,t-1)}{k^M_{P_+}(x,y_0,t)}=1,\quad\text{and}\quad \lim_{t\to\infty}\frac{k^M_{P_0}(x,y_0,t+1)}{k^M_{P_0}(x,y_0,t)}=1\qquad\forall x\in M. \tag{8.12}$$

Therefore, (8.11) and (8.12) imply that there exists $C_0>0$ such that

$$k^M_{P_+}(x,y_0,t)\le C_0k^M_{P_0}(x,y_0,t)\qquad \forall x\in M, t>T(x). \tag{8.13}$$

Consequently, (8.10) and (8.13) imply that

$$u_+(x)\le C_0u_0(x)=\tilde{C}_0\varphi(x)\qquad \forall x\in M.$$

Therefore, using (8.4) we obtain

$$(u_+)^2(x)m_+(x)A_+(x)\le C_2\varphi^2(x)m_0(x)A_0(x)\qquad \text{for a.e. } x\in M, \tag{8.14}$$

where $C_2>0$ is a positive constant. Thus, Theorem 2.11 implies that P_+ is critical in M which is a contradiction. The last statement of the theorem follows from the parabolic Harnack inequality and parabolic regularity. □

By the generalized maximum principle, assumption (8.5) in Theorem 8.4 is satisfied with $C=1$ if $P_+=P_0+V$, where P_0 is a critical operator on M and V is any *nonnegative* potential. Note that if the potential is in addition nontrivial, then P_+ is indeed subcritical in M. Therefore, we have

Corollary 8.5 ([24]). *Let P_0 be a symmetric operator of the form* (8.3) *which is critical in M, and let $P_+:=P_0+V_1$, where V_1 is a nonzero nonnegative potential. Then*

$$\lim_{t\to\infty}\frac{k^M_{P_+}(x,y,t)}{k^M_{P_0}(x,y,t)}=0 \tag{8.15}$$

locally uniformly in $M\times M$.

Next, we discuss the nonsymmetric case. We study two cases where Davies' conjecture implies Conjecture 8.1. First, we show that in the nonsymmetric case, the result of Corollary 8.5 for positive perturbations of a critical operator P_0 still holds provided that the validity of Davies' conjecture (Conjecture 7.1) is assumed instead of the symmetry hypothesis. More precisely, we have

Theorem 8.6 ([24]). *Let P_0 be a critical operator in M, and let $P_+ = P_0 + V$, where V is any nonzero nonnegative potential on M. Assume that Davies' conjecture (Conjecture 7.1) holds true for both $k_{P_0}^M$ and $k_{P_+}^M$. Then*

$$\lim_{t\to\infty} \frac{k_{P_+}^M(x,y,t)}{k_{P_0}^M(x,y,t)} = 0 \tag{8.16}$$

locally uniformly in $M \times M$.

Proof. Recall that in light of Remark 8.2 we assume that $\lambda_0(P_+, M) = 0$. Suppose to the contrary that for some $x_0, y_0 \in M$ there exists a sequence $\{t_n\}$ such that $t_n \to \infty$ and

$$\lim_{n\to\infty} \frac{k_{P_+}^M(x_0,y_0,t_n)}{k_{P_0}^M(x_0,y_0,t_n)} = K > 0. \tag{8.17}$$

Consider the functions v_+ and v_0 defined by

$$v_+(x,t) := \frac{k_{P_+}^M(x,y_0,t)}{k_{P_+}^M(x_0,y_0,t)}, \quad v_0(x,t) := \frac{k_{P_0}^M(x,y_0,t)}{k_{P_0}^M(x_0,y_0,t)} \qquad x \in M, t > 0.$$

By our assumption,

$$\lim_{t\to\infty} v_+(x,t) = u_+(x), \qquad \lim_{t\to\infty} v_0(x,t) = u_0(x),$$

where $u_+ \in \mathcal{C}_{P_+}(M)$ and $u_0 \in \mathcal{C}_{P_0}(M)$.

On the other hand, by the generalized maximum principle

$$\frac{k_{P_+}^M(x,y_0,t)}{k_{P_0}^M(x,y_0,t)} \leq 1. \tag{8.18}$$

Therefore,

$$\frac{k_{P_+}^M(x_0,y_0,t_n)}{k_{P_0}^M(x_0,y_0,t_n)} \times \frac{\frac{k_{P_+}^M(x,y_0,t_n)}{k_{P_+}^M(x_0,y_0,t_n)}}{\frac{k_{P_0}^M(x,y_0,t_n)}{k_{P_0}^M(x_0,y_0,t_n)}} = \frac{k_{P_+}^M(x,y_0,t_n)}{k_{P_0}^M(x,y_0,t_n)} \leq 1. \tag{8.19}$$

Letting $n \to \infty$ we obtain

$$Ku_+(x) \leq u_0(x) \qquad x \in M. \tag{8.20}$$

It follows that $v(x) := u_0(x) - Ku_+(x)$ is a nonnegative supersolution of the equation $P_0 u = 0$ in M which is not a solution. In particular, $v \neq 0$. By the strong maximum principle $v(x)$ is a strictly positive supersolution of the equation $P_0 u = 0$ in M which is not a solution. This contradicts the criticality of P_0 in M. $\square$

The second nonsymmetric result concerns semismall perturbations.

Theorem 8.7 ([24]). *Let P_+ and $P_0 = P_+ + V$ be a subcritical operator and a critical operator in M, respectively. Suppose that V is a semismall perturbation of the operator P_+^* in M. Assume further that Davies' conjecture (Conjecture 7.1) holds true for both $k_{P_0}^M$ and $k_{P_+}^M$ and that (8.5) holds true. Then*

$$\lim_{t\to\infty} \frac{k_{P_+}^M(x,y,t)}{k_{P_0}^M(x,y,t)} = 0 \tag{8.21}$$

locally uniformly in $M \times M$.

Proof. Recall that we (may) assume that $\lambda_0(P_+, M) = 0$. Assume to the contrary that for some $x_0, y_0 \in M$ there exists a sequence $\{t_n\}$ such that $t_n \to \infty$ and

$$\lim_{n\to\infty} \frac{k_{P_+}^M(x_0,y_0,t_n)}{k_{P_0}^M(x_0,y_0,t_n)} = K > 0. \tag{8.22}$$

Consider the functions v_+ and v_0 defined by

$$v_+(x,t) := \frac{k_{P_+}^M(x,y_0,t)}{k_{P_+}^M(x_0,y_0,t)}, \quad v_0(x,t) := \frac{k_{P_0}^M(x,y_0,t)}{k_{P_0}^M(x_0,y_0,t)} \qquad x \in M, t > 0. \tag{8.23}$$

By our assumption,

$$\lim_{t\to\infty} v_+(x,t) = u_+(x), \qquad \lim_{t\to\infty} v_0(x,t) = u_0(x),$$

where $u_+ \in \mathcal{C}_{P_+}(M)$ and $u_0 \in \mathcal{C}_{P_0}(M)$.

On the other hand, by assumption (8.5) we have for $t > T(x)$

$$\frac{k_{P_+}^M(x,y_0,t)}{k_{P_0}^M(x,y_0,t)} = \frac{k_{P_+}^M(x,y_1,t)}{k_{P_0}^M(x,y_1,t)} \times \frac{\frac{k_{P_+}^M(x,y_0,t)}{k_{P_+}^M(x,y_1,t)}}{\frac{k_{P_0}^M(x,y_0,t)}{k_{P_0}^M(x,y_1,t)}} \leq C \frac{k_{P_+}^M(x,y_0,t)}{k_{P_+}^M(x,y_1,t)} \times \frac{k_{P_0}^M(x,y_1,t)}{k_{P_0}^M(x,y_0,t)}. \tag{8.24}$$

By our assumption on Davies' conjecture, we have for a fixed x

$$\lim_{t\to\infty} \frac{k_{P_+}^M(x,y_0,t)}{k_{P_+}^M(x,y_1,t)} = \frac{u_+^*(y_0)}{u_+^*(y_1)}, \qquad \lim_{t\to\infty} \frac{k_{P_0}^M(x,y_1,t)}{k_{P_0}^M(x,y_0,t)} = \frac{u_0^*(y_1)}{u_0^*(y_0)}, \tag{8.25}$$

where u_+^* and u_0^* are positive solutions of the equation $P_+^* u = 0$ and $P_0^* u = 0$ in M, respectively. By the elliptic Harnack inequality there exists a positive constant C_1 (depending on P_+^*, P_0^*, y_0, y_1 but not on x) such that

$$\frac{u_+^*(y_0)}{u_+^*(y_1)} \leq C_1, \qquad \frac{u_0^*(y_1)}{u_0^*(y_0)} \leq C_1. \tag{8.26}$$

Therefore, (8.24) and (8.26) imply that

$$\frac{k_{P_+}^M(x,y_0,t_n)}{k_{P_0}^M(x,y_0,t_n)} \leq 2CC_1^2 \tag{8.27}$$

for n sufficiently large (which might depend on x).

Therefore,

$$\frac{k_{P_+}^M(x_0,y_0,t_n)}{k_{P_0}^M(x_0,y_0,t_n)} \times \frac{\frac{k_{P_+}^M(x,y_0,t_n)}{k_{P_+}^M(x_0,y_0,t_n)}}{\frac{k_{P_0}^M(x,y_0,t_n)}{k_{P_0}^M(x_0,y_0,t_n)}} = \frac{k_{P_+}^M(x,y_0,t_n)}{k_{P_0}^M(x,y_0,t_n)} \leq 2CC_1^2\,. \tag{8.28}$$

Letting $n \to \infty$ and using (8.22) and (8.23), we obtain

$$Ku_+(x) \leq 2CC_1^2 u_0(x) \qquad x \in M\,. \tag{8.29}$$

On the other hand, since V is a semismall perturbation of P_+^* in M, Theorem 2.13 implies that $u_0(x) \asymp G_{P_+}^M(x,y_0)$ in $M \setminus \overline{B(y_0,\delta)}$, with some positive δ. Consequently,

$$u_+(x) \leq C_2 G_{P_+}^M(x,y_0) \qquad x \in M \setminus \overline{B(y_0,\delta)} \tag{8.30}$$

for some $C_2 > 0$. In other words, u_+ is a global positive solution of the equation $P_+u = 0$ in M which has minimal growth in a neighborhood of infinity in M. Therefore u_+ is a ground state of the equation $P_+u = 0$ in M, but this contradicts the subcriticality of P_+ in M. □

9. On the equivalence of heat kernels

In this section we study a general question concerning the equivalence of heat kernels which in turn will give sufficient conditions for the validity of the boundedness condition (8.5) that is assumed in Theorems 8.4 and 8.7.

Definition 9.1. *Let P_i, $i = 1,2$, be two elliptic operators of the form* (2.1) *that are defined on M and satisfy $\lambda_0(P_i, M) = 0$ for $i = 1,2$. We say that the heat kernels $k_{P_1}^M(x,y,t)$ and $k_{P_2}^M(x,y,t)$ are* equivalent (*respectively,* semiequivalent) *if*

$$k_{P_1}^M \asymp k_{P_2}^M \qquad \text{on } M \times M \times (0,\infty)$$

(*respectively,* $k_{P_1}^M(\cdot,y_0,\cdot) \asymp k_{P_2}^M(\cdot,y_0,\cdot)$ *on* $M \times (0,\infty)$ *for some fixed* $y_0 \in M$).

There is an intensive literature dealing with (almost optimal) conditions under which two positive (minimal) Green functions are equivalent or semiequivalent (see [3, 43, 46, 50] and the references therein). On the other hand, sufficient conditions for the equivalence of heat kernels are known only in a few cases (see [39, 40, 67]). In particular, it seems that the answer to the following conjecture is not known.

Conjecture 9.2 ([24]). *Let P_1 and P_2 be two subcritical operators of the form* (2.1) *that are defined on a Riemannian manifold M such that $P_1 = P_2$ outside a compact set in M, and $\lambda_0(P_i, M) = 0$ for $i = 1,2$. Then $k_{P_1}^M$ and $k_{P_2}^M$ are equivalent.*

Remark 9.3. Suppose that P_1 and P_2 satisfy the assumption of Conjecture 9.2. B. Devyver and the author proved recently that there exists $C > 0$ such that

$$C^{-1}G_{P_2-\lambda}^M(x,y) \leq G_{P_1-\lambda}^M(x,y) \leq CG_{P_2-\lambda}^M(x,y) \quad \forall x,y \in M, \text{ and } \lambda \leq 0. \tag{9.1}$$

Clearly, by (1.7), the above estimate (9.1) is a necessary condition for the validity of Conjecture 9.2.

It is well known that certain 3-G inequalities imply the equivalence of Green functions, and the notions of small and semismall perturbations is based on this fact. Moreover, small (respectively, semismall) perturbations are sufficient conditions and in some sense also necessary conditions for the equivalence (respectively, semiequivalence) of the Green functions [43, 46, 50]. Therefore, it is natural to introduce an analog definition for heat kernels (cf. [67]).

Definition 9.4. Let P be a subcritical operator in M. We say that a potential V is a *k-bounded perturbation* (respectively, *k-semibounded perturbation*) with respect to the heat kernel $k_P^M(x,y,t)$ if there exists a positive constant C such that the following 3-k inequality is satisfied:

$$\int_0^t \int_M k_P^M(x,z,t-s)|V(z)|k_P^M(z,y,s)\,\mathrm{d}z\,\mathrm{d}s \le Ck_P^M(x,y,t) \tag{9.2}$$

for all $x,y \in M$ (respectively, for a fixed $y \in M$, and all $x \in M$) and $t>0$.

The following result shows that the notion of k-(semi)boundedness is naturally related to the (semi)equivalence of heat kernels.

Theorem 9.5 ([24]). *Let P be a subcritical operator in M, and assume that the potential V is k-bounded perturbation (respectively, k-semibounded perturbation) with respect to the heat kernel $k_P^M(x,y,t)$. Then there exists $c>0$ such that for any $|\varepsilon|<c$ the heat kernels $k_{P+\varepsilon V}^M(x,y,t)$ and $k_P^M(x,y,t)$ are equivalent (respectively, semiequivalent).*

Proof. Consider the iterated kernels

$$k_P^{(j)}(x,y,t) := \begin{cases} k_P^M(x,y,t) & j=0,\\ \int_0^t\int_M k_P^{(j-1)}(x,z,t-s)V(z)k_P^M(z,y,s)\,\mathrm{d}z\,\mathrm{d}s & j\ge 1. \end{cases}$$

Using (9.2) and an induction argument, it follows that

$$\sum_{j=0}^{\infty}|\varepsilon|^j|k_P^{(j)}(x,y,t)| \le \left(1+C|\varepsilon|+C^2|\varepsilon|^2+\cdots\right)k_P^M(x,y,t) = \frac{1}{1-C|\varepsilon|}\,k_P^M(x,y,t)$$

provided that $|\varepsilon|<C^{-1}$. Consequently, for such ε the Neumann series

$$\sum_{j=0}^{\infty}(-\varepsilon)^j k_P^{(j)}(x,y,t)$$

converges locally uniformly in $M\times M\times\mathbb{R}_+$ to $k_{P+\varepsilon V}^M(x,y,t)$ which in turn implies that Duhamel's formula

$$k_{P+\varepsilon V}^M(x,y,t) = k_P^M(x,y,t) - \varepsilon\int_0^t\int_M k_P^M(x,z,t-s)V(z)k_{P+\varepsilon V}^M(z,y,s)\,\mathrm{d}z\,\mathrm{d}s \tag{9.3}$$

is valid. Moreover, we have

$$k^M_{P+\varepsilon V}(x,y,t) \le \frac{1}{1-C|\varepsilon|}\, k^M_P(x,y,t).$$

The lower bound

$$C_1 k^M_P(x,y,t) \le k^M_{P+\varepsilon V}(x,y,t)$$

(for $|\varepsilon|$ small enough) follows from the upper bound using (9.3) and (9.2). □

Corollary 9.6 ([24]). *Assume that P and V satisfy the conditions of Theorem 9.5, and suppose further that V is nonnegative. Then there exists $c > 0$ such that for any $\varepsilon > -c$ the heat kernels $k^M_{P+\varepsilon V}(x,y,t)$ and $k^M_P(x,y,t)$ are equivalent (respectively, semiequivalent).*

Proof. By Theorem 9.5 the heat kernels $k^M_{P+\varepsilon V}(x,y,t)$ and $k^M_P(x,y,t)$ are equivalent (respectively, semiequivalent) for any $|\varepsilon| < c$.

Recall that by the generalized maximum principle,

$$k^M_{P+\varepsilon V}(x,y,t) \le k^M_P(x,y,t) \qquad \forall \varepsilon > 0. \tag{9.4}$$

On the other hand, given a potential W (not necessarily of definite sign), and $0 \le \alpha \le 1$, denote $P_\alpha := P + \alpha W$, and assume that $P_j \ge 0$ in M for $j = 0, 1$. Then for $0 \le \alpha \le 1$ we have $P_\alpha \ge 0$ in M, and the following inequality holds [47]

$$k^M_{P_\alpha}(x,y,t) \le [k^M_{P_0}(x,y,t)]^{1-\alpha}[k^M_{P_1}(x,y,t)]^{\alpha} \qquad \forall\, x,y \in M,\ t > 0. \tag{9.5}$$

Using (9.4) and (9.5) we obtain the desired equivalence $k^M_{P+\varepsilon V} \asymp k^M_P$ also for $\varepsilon \ge c$. □

Finally we have:

Theorem 9.7 ([24]). *Let P_0 be a critical operator in M. Assume that $V = V_+ - V_-$ is a potential such that $V_\pm \ge 0$ and $P_+ := P_0 + V$ is subcritical in M.*

Assume further that V_- is k-semibounded perturbation with respect to the heat kernel $k^M_{P_+}(x,y_1,t)$. Then condition (8.5) is satisfied uniformly in x. That is, there exist positive constants C and T such that

$$k^M_{P_+}(x,y_1,t) \le C k^M_{P_0}(x,y_1,t) \qquad \forall x \in M, t > T. \tag{9.6}$$

Proof. By Corollary 9.6, the heat kernels $k^M_{P_+}(x,y_1,t)$ and $k^M_{P_++V_-}(x,y_1,t)$ are semiequivalent. Note that $P_+ + V_- = P_0 + V_+$. Therefore we have

$$\begin{aligned} C^{-1}k^M_{P_+}(x,y_1,t) &\le k^M_{P_++V_-}(x,y_1,t) \\ &= k^M_{P_0+V_+}(x,y_1,t) \le k^M_{P_0}(x,y_1,t) \quad \forall x \in M, t > 0. \end{aligned}$$ □

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