Mathematical aspects of quantum mechanics with non-self-adjoint operators

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Résumé

The thesis is aiming at mathematical studies of problems coming from the new concept in quantum mechanics where observables are represented by non-self-adjoint operators. We focus on criteria of similarity of non-self-adjoint unbounded operators to self-adjoint and normal operators and the structure of the similarity transforms; and on spectral and psudospectral properties of Schrödinger operators with complex potentials and non-self-adjoint boundary conditions.

The main achievements are represented by new models for which the similarity transforms can be found in a closed form; by the proof of absence of Riesz basis property for the imaginary cubic oscillator and other paradigmatic models in physics theories; by the development of theory of quantum graphs with non-self-adjoint boundary conditions together with a new classification; and by a first systematic and general non-semi-classical approach for the construction of pseudomodes of Schrödinger operators with complex potentials.

To my children,
Václav, Antonín Boleslav and Vojtěch Podiven

Studying non-self-adjoint 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.

E. B. Davies, *Linear operators and their spectra* (Cambridge 2007)

Contents

Preface

At the turn of the millennium, physicists came up with the idea to extend quantum mechanics by considering observables represented by non-self-adjoint operators. The rapid advance of the subject since that date is reflected in the exponential growth of articles by distinct research groups throughout the world published in prestigious physics journals, including *Nature* and *Physical Review Letters*. It is striking that this non-self-adjoint representation was overlooked for almost 100 years since the advent of quantum mechanics and it unquestionably deserves a serious attention from the scientific community.

Unfortunately, the heuristic approach of the majority of the physics works reveals a vast area of statements that are unjustified on a rigorous level and often leads to paradoxes and puzzling discussions among the various research groups involved. The principal objective of this thesis is to contribute to the new area of physics by providing a mathematically rigorous approach for a correct implementation of the interesting idea and by resolving some of the puzzlements with help of standard as well as unconventional methods of modern operator theory. More generally, the thesis is concerned with spectral theory of non-self-adjoint differential operators.

The core of the thesis is formed by my research articles published on the topic since 2006. In view of my distinct focuses on various aspects of quantum mechanics with non-self-adjoint operators in the recent years, in this thesis I divide the articles into the following key groups:

I. toy models,

II. waveguides,

III. pseudospectra.

***ad* I.** Motivated by the needs of nuclear physics, Scholtz, Geyer and Hahne suggested in 1992 [59] an interesting representation of observables in quantum mechanics by operators which are not necessarily self-adjoint but merely *quasi-self-adjoint*, that is, similar to self-adjoint operators. Then it is enough to change the inner product in the underlying Hilbert space with help of a *metric* operator obviously related to the similarity transform. The interest in this class of operators was renewed in 1998 when Bender *et al.* [6] suggested that a large class of non-self-adjoint operators possess real spectra as a consequence of an antilinear parity-time ($\mathcal{PT}$) symmetry. However, it is not easy to decide whether a non-self-adjoint operator is quasi-self-adjoint. In fact, only a few examples were available in the physics literature at that time and, moreover, the majority of the approaches were mathematically unjustifiable constructions based on formal infinite series of unbounded operators.

The lack of simple rigorous models was the main motivation for me to enter the research field in 2006 with a paper [39] (Chapter 3), in which we introduce a very simple $\mathcal{PT}$-symmetric Sturm-Liouville-type operator and establish a *closed formula* for the metric. This formula is further simplified in [36] (Chapter 4). In [46] (Chapter 5) we eventually succeed to write down also the self-adjoint counterpart as a simple albeit non-local operator and study the problem in a more general context. A physical interpretation of the model in terms of scattering is given in [27] (Chapter 6). Finally, in [42] (Chapter 7) and [33] (Chapter 8) we extend the model to curved manifolds and operator matrices of Pauli type, respectively.

In [34] (Chapter 9) we employ the notion of quasi-self-adjointness to explain the reality of the spectrum of the generator of a stochastic process modelling the Brownian motion with random jumps from the boundary. Here the problem is not originally quantum-mechanical, but the tools are motivated by the new concept in quantum mechanics.

The title "toy models" of group I essentially means "one-dimensional models". I include in it also a more general class of models of [29] (Chapter 10), where we develop a systematic study of the Laplacian on finite metric graphs, subject to various classes of non-self-adjoint boundary conditions imposed at graph vertices. Among other things, we describe a simple way to relate the similarity transforms between Laplacians on certain graphs with elementary similarity transforms between matrices defining the boundary conditions.

***ad* II.** The simplicity of the toy model of [39] is due to the fact that the non-self-adjoint operator is just the one-dimensional Laplacian in a bounded interval, subject to *complex Robin boundary conditions*. In [11] (Chapter 11) we make the problem richer by considering this type of $\mathcal{PT}$-symmetric boundary conditions, not necessarily homogeneous now, on a two-dimensional infinite strip. We show that the essential spectrum is real, establish sufficient conditions which guarantee the existence of real discrete spectra and compute weak-coupling asymptotics of the corresponding eigenvalues. Further spectral results are established in [47] (Chapter 12) with help of numerical simulations. In particular, it turns out that the spectrum is not always real, but there might be complex-conjugate eigenvalues for large values of a boundary-coupling parameter. In an invited open-problem note [38] (Chapter 13) we point out the need for a robust method establishing the existence of isolated eigenvalues for non-self-adjoint operators possessing an essential spectrum.

In [12] (Chapter 14) we extend the model of [11] to higher dimensions and derive an effective (self-adjoint) operator to which the non-self-adjoint Robin Laplacian converges in a norm-resolvent sense when the width of the hyper-strip tends to zero. A generalisation of this result to tubular neighbourhoods of curved hypersurfaces in a much more general context is given in [41] (Chapter 15).

In [35] (Chapter 16) we consider another type of model, where the non-self-adjoint operator is the Laplacian in the whole Euclidean space of any dimension with a *complex delta interaction* supported by two parallel hypersurfaces. We analyse spectral properties of the system in the limit when the distance between the hypersurfaces tends to zero.

In [20] (Chapter 17) we establish the absence of point spectra for electromagnetic Schrödinger operators with complex electric potentials under various conditions and by two different methods: the Birman-Schwinger principle and the method of multipliers. Finally, in [40] (Chapter 18) we introduce a closed Dirichlet realisation of non-accretive electromagnetic Schrödinger operators with complex electric potentials on arbitrary open sets and show that the eigenfunctions corresponding to discrete eigenvalues satisfy an Agmon-type exponential decay.

The title “waveguides” of part II is a bit artificial. In particular, the geometrical setting of [41] is much more general, while there is no tubular geometry in [20]. The common point of the papers in part II is that the models are higher dimensional, the operators possess an essential spectrum, there is a non-trivial interaction due to complex fields or boundary conditions and the emphasis is put on spectral properties.

***ad* III.** The most significant contribution – at least from the point of view of impact and the acceptance by the community – is probably contained in part III. Here we group together our papers in which the mathematical concept of *pseudospectra* as the right tool to capture and rigorously describe non-self-adjoint features of the $\mathcal{PT}$-symmetric and other non-self-adjoint operators considered in the physics literature in recent years was suggested.

In [61] (Chapter 19) we show that the eigenfunctions of the imaginary cubic oscillator, which has been considered as the *fons et origo* of $\mathcal{PT}$-symmetric quantum mechanics, are complete but do not form a Riesz basis. This results in the existence of a bounded metric operator having intrinsic singularity reflected in the inevitable unboundedness of the inverse. Consequently, the model is not relevant quantum-mechanically as a representative of a physical observable. The proof is based on a semiclassical construction of pseudomodes. This concise paper written for the physics community is followed by a more detailed survey [45] (Chapter 20), in which the concept of pseudospectra is suggested in the context of quasi-self-adjointness in quantum mechanics with many concrete examples.

In [26] (Chapter 21) we develop a spectral and pseudospectral analysis of the Schrödinger operator with an imaginary sign potential on the real line. It turns out that the pseudospectra of this operator are highly non-trivial. One of the interests of the paper [26] is due to the fact that it cannot be turned to a semiclassical operator and, moreover, the semiclassical construction of pseudomodes requires that the potential is at least continuous. In view of this lack of semiclassical tools, in the most recent paper [44] (Chapter 22) we develop a first systematic and very general non-semi-classical approach for the construction of pseudomodes of Schrödinger operators with complex potentials.

This thesis may be considered as a research report mostly based on the aforementioned papers of the author obtained in the last few years. On the other hand, in the following introductory Chapter 1, we provide a concise summary of the new concept of quasi-self-adjointness in quantum mechanics and review the basic material which is needed. Furthermore, in Chapter 2, we give a brief and intentionally informal summary of the main results obtained in the papers. In this sense we believe that the two chapters represent a self-contained treatment of the recent research, accessible to non-specialists and, in particular, to students interested in the topics where functional analysis (especially spectral theory) meets quantum mechanics.

The thesis thus consists of four main parts. Part 0 consists of the two introductory Chapters 1–2, while Parts I–III (Chapters 3–22) contain the published material as described above. At the end of the document, we add Appendix A which is a book chapter [43] summarising some standard material from operator theory in the context of quasi-self-adjoint quantum mechanics.

For the convenience of the reader, we present here the publications on which the thesis is based:

Chapter 3 D. Krejčiřík, H. Bíla, and M. Znojil, *Closed formula for the metric in the Hilbert space of a $\mathcal{PT}$-symmetric model*, J. Phys. A **39** (2006), 10143–10153.

Chapter 4 D. Krejčiřík, *Calculation of the metric in the Hilbert space of a $\mathcal{PT}$-symmetric model via the spectral theorem*, J. Phys. A: Math. Theor. **41** (2008), 244012.

Chapter 5 D. Krejčiřík, P. Siegl, and Železný, *On the similarity of Sturm-Liouville operators with non-Hermitian boundary conditions to self-adjoint and normal operators*, Complex Anal. Oper. Theory **8** (2014), 255–281.

Chapter 6 H. Hernandez-Coronado, D. Krejčiřík, and P. Siegl, *Perfect transmission scattering as a $\mathcal{PT}$-symmetric spectral problem*, Phys. Lett. A **375** (2011), 2149–2152.

Chapter 7 D. Krejčiřík and P. Siegl, *$\mathcal{PT}$-symmetric models in curved manifolds*, J. Phys. A: Math. Theor. **43** (2010), 485204.

Chapter 8 D. Kochan, D. Krejčiřík, R. Novák, and P. Siegl, *The Pauli equation with complex boundary conditions*, J. Phys. A: Math. Theor. **45** (2012), 444019.

Chapter 9 M. Kolb and D. Krejčiřík, *Spectral analysis of the diffusion operator with random jumps from the boundary*, Math. Z. **284** (2016), 877–900.

Chapter 10 A. Hussein, D. Krejčiřík, and P. Siegl, *Non-self-adjoint graphs*, Trans. Amer. Math. Soc. **367** (2015), 2921–2957.

Chapter 11 D. Borisov and D. Krejčiřík, *$\mathcal{PT}$-symmetric waveguides*, Integ. Equ. Oper. Theory **62** (2008), 489–515.

Chapter 12 D. Krejčiřík and M. Tater, *Non-Hermitian spectral effects in a $\mathcal{PT}$-symmetric waveguide*, J. Phys. A: Math. Theor. **41** (2008), 244013.

Chapter 13 D. Krejčiřík, *$\mathcal{PT}$-symmetric waveguides and the lack of variational techniques*, Integral Equations Operator Theory **73** (2012), 1–2.

Chapter 14 D. Borisov and D. Krejčiřík, *The effective Hamiltonian for thin layers with non-Hermitian Robin-type boundary conditions*, Asympt. Anal. **76** (2012), 49–59.

Chapter 15 D. Krejčiřík, N. Raymond, J. Royer, and P. Siegl, *Reduction of dimension as a consequence of norm-resolvent convergence and applications*, arXiv:1701.08819 [math-ph] (2017).

Chapter 16 S. Kondej and D. Krejčiřík, *Asymptotic spectral analysis in colliding leaky quantum layers*, J. Math. Anal. Appl. **446** (2017), 1328–1355.

Chapter 17 L. Fanelli, D. Krejčiřík, and L. Vega, *Spectral stability of Schrödinger operators with subordinated complex potentials*, J. Spectr. Theory, to appear.

Chapter 18 D. Krejčiřík, N. Raymond, J. Royer, and P. Siegl, *Non-accretive Schrödinger operators and exponential decay of their eigenfunctions*, Israel J. Math., to appear.

Chapter 19 P. Siegl and D. Krejčiřík, *On the metric operator for the imaginary cubic oscillator*, Phys. Rev. D **86** (2012), 121702(R).

Chapter 20 D. Krejčiřík, P. Siegl, M. Tater, and J. Viola, *Pseudospectra in non-Hermitian quantum mechanics*, J. Math. Phys. **56** (2015), 103513.

Chapter 21 R. Henry and D. Krejčiřík, *Pseudospectra of the Schrödinger operator with a discontinuous complex potential*, J. Spectr. Theory, to appear.

Chapter 22 D. Krejčiřík and P. Siegl, *Pseudomodes for Schrödinger operators with complex potentials*, arXiv:1705.01894 [math.SP] (2017).

Appendix A D. Krejčiřík and P. Siegl, *Elements of spectral theory without the spectral theorem*, In *Non-selfadjoint operators in quantum physics: Mathematical aspects* (432 pages), F. Bagarello, J.-P. Gazeau, F. H. Szafraniec, and M. Znojil, Eds., Wiley-Interscience, 2015.

Except for unifying cosmetical amendments, the contents of Chapters 3–22 and Appendix A coincide with the published versions of the building papers and book chapter. This decision leads to two counter effects. First, the notation introduced in Part 0 (Chapters 1–2) may occasionally differ from that used in the individual articles presented in Parts I–III (Chapters 3–22) and Appendix A. This is balanced by the fact that each of the Chapters 3–22 and Appendix A can be read as an independent research work, in its original version. Second, more importantly, we decided not to correct misprints and possible mistakes we have encountered after the publication of some of the papers and the book chapter. *Errare humanum est.* In fact, we are aware of just a few cases, which are treated in this thesis by adding a short errata section after the list of references of the corresponding chapter.

The present thesis is thematically orthogonal to my *Doctor of Science* (DSc) thesis [37], defended in 2012, which was formed by my articles in spectral geometry and thus essentially self-adjoint. None of the papers of my DSc thesis is presented in this thesis. At the same time, my other recent articles which do not fit into the present subject are not included in this thesis either.

I conclude by thanking the large number of people who have stimulated my interest in quantum mechanics with non-self-adjoint operators over the last fifteen years, particularly in relation to the content of this thesis. The most important of these has been Petr Siegl, my principal co-author and a good friend, who moreover read a previous version of this thesis and offered invaluable comments. I am also very grateful to my other co-authors from the above papers and to many other good friends and colleagues. I am particularly indebted to Miloslav Znojil whose persistence eventually made me become involved in non-self-adjoint spectral theory. Finally I want to record my thanks to my wife and our children; I would never have been able to write this thesis without their support.

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Part 0

Introductory part

Chapter 1

Introduction

1.1 Physical motivations

Many physical systems can be described by partial differential equations and the latter can often be viewed as generating abstract operators between Banach spaces. A typical example is quantum mechanics, where the state of the system is described by a vector ψ in a Hilbert space and its time evolution is governed by the Schrödinger equation

$$i\,\frac{\partial\psi}{\partial t} = H\psi \tag{1.1}$$

with H being a linear *self-adjoint* operator (so-called Hamiltonian) representing the total energy of the system. In other areas of physics a more general class of operators is necessary to describe a process in Nature, where the non-self-adjointness is typically related to non-conservative phenomena like for instance dissipation. In this thesis, we almost exclusively focus on the role of non-self-adjoint operators in quantum mechanics, which is an intrinsically conservative theory because the solution of (1.1) is clearly given by the *unitary* group

$$e^{-itH} \tag{1.2}$$

applied to an initial state. Hence the following question may seem to be an odd kind of connection:

Can quantum theory be extended by *non-self-adjoint* operators playing the role of observables?

This question is both tempting and misleading. First of all, it is important that the non-self-adjointness is restricted to observables, because in different contexts quantum mechanics is in fact full of non-self-adjoint operators. Indeed, the resolvent of H for complex energies so as the propagator (1.2) are non-self-adjoint operators, but here the non-self-adjointness is unimportant because these examples are obtained as functions of self-adjoint operators. More importantly, non-self-adjoint operators play an important role in topics as diverse as the solution of the spectral problem for the harmonic oscillator via the creation and annihilation operators, study of resonances by the method of complex scaling and the effective models for dynamics of open systems. However, the non-self-adjointness arises there as a result of a technical method or a useful approximation to attack a concrete physical problem involving observables correctly described by self-adjoint operators.

The question above is tempting because, naïvely, an "extension" of quantum theory might potentially cover processes in Nature that we are currently unable to explain via "standard" quantum mechanics. Here we use quotation marks because quantum theory is intrinsically conservative and it is a well known mathematical fact (Stone's theorem) that generators of unitary groups are *necessarily* self-adjoint operators. That is why the question above is misleading and the subject of the present thesis might be regarded as inappropriate at this point.

Adopting a less fundamental approach, however, the question above can be given an affirmative answer. This is the content of the so-called *quasi-Hermitian quantum mechanics* that we explain now.

1.1.1 Quasi-Hermitian quantum mechanics

Motivated by the needs of nuclear physics, in 1992 F. G. Scholtz, H. B. Geyer and F. J. W. Hahne [59] came up with the idea that a consistent (conventional) quantum-mechanical interpretation holds for an observable represented by a non-self-adjoint operator H, provided that it satisfies the *quasi-Hermitian* relation

$$H^* = \Theta H \Theta^{-1} \tag{1.3}$$

with some positive, bounded and boundedly invertible operator Θ called *metric* and the inner product $\langle\cdot,\cdot\rangle$ in the underlying Hilbert space is simultaneously modified to $\langle\cdot,\Theta\,\cdot\rangle$. That is, like in Einsteins theory of relativity, there is an intertwining relationship between the space and its constituents.

Notice that the special choice $\Theta = I$ in (1.3) corresponds to H being self-adjoint, *i.e.* $H^* = H$. An operator H satisfying (1.3) with a general positive, bounded and boundedly invertible operator Θ will be called *quasi-self-adjoint* in this thesis. It is easy to see that H is quasi-self-adjoint if, and only if, it is *similar* to a self-adjoint operator, *i.e.* there exists a self-adjoint operator h and a bounded and boundedly invertible operator Ω such that

$$h = \Omega H \Omega^{-1}\,. \tag{1.4}$$

Indeed, if H satisfies (1.3), then h from (1.4) is self-adjoint provided that we set $\Omega := \Theta^{1/2}$. Vice versa, an operator H satisfying (1.4) is quasi-self-adjoint with $\Theta := \Omega^*\Omega$.

Summing up, a consistent quantum mechanics can be built for an observable represented by a non-self-adjoint operator provided the latter is similar to a self-adjoint operator. Let us stress that the concept of quasi-self-adjointness is by no means any extension of quantum mechanics, it is just a non-standard (and potentially useful) representation.

The concept of operators satisfying the type of relations (1.3) was previously considered by the mathematician J. Dieudonné in 1961 [18]. It is surprising that the quasi-self-adjoint representation of observables was overlooked for so many years since the foundations of quantum mechanics and it is even more surprising that the more recent physically motivated work [59] did not attract enough attention from the scientific community shortly after its appearance. In fact, the strong impetus to consider quasi-self-adjoint operators in quantum mechanics came only after the advent of another new concept of physicists: $\mathcal{PT}$-*symmetric quantum mechanics*.

1.1.2 $\mathcal{PT}$-symmetric quantum mechanics

In 1998 C. M. Bender and P. N. Boetcher [6] noticed that a large class of operators possess real spectra as a consequence of certain physical-like antilinear symmetries instead of the self-adjointness and suggested extending quantum mechanics by these operators. For Schrödinger operators $-\Delta+V$ in $L^2(\mathbb{R}^d)$ with $V:\mathbb{R}^d\to\mathbb{C}$, the considered symmetry means the commutation relation

$$[H,\mathcal{PT}] = 0\,, \tag{1.5}$$

where $(\mathcal{P}\psi)(x) := \psi(-x)$ is the linear *space-reversal* or *parity* operator and $(\mathcal{T}\psi)(x) := \overline{\psi(x)}$ is the antilinear *time-reversal* operator (notice that the time reversal $t\mapsto -t$ is equivalent to the complex conjugation $i\mapsto -i$ in the context of scalar Schrödinger equation (1.1)).

The paradigmatic example of [6] was the *imaginary cubic oscillator* (sometimes also referred to as *Bender's oscillator*)

$$-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + ix^3 \qquad \text{in} \qquad L^2(\mathbb{R})\,. \tag{1.6}$$

The arguments of [6] were actually based on a numerical study of eigenvalues of (1.6) and other one-dimensional Schrödinger operators with polynomial $\mathcal{PT}$-symmetric potentials. The proof that the eigenvalues of (1.6) are indeed real was provided by P. Dorey, C. Dunning and R. Tateo in 2001 [19] (see also [60] and [22]).

In a series of papers from the period 2002–2003 [50, 51, 52], A. Mostafazadeh suggested that the correct implementation of $\mathcal{PT}$-symmetric operators in quantum mechanics should be given through the previously introduced concept of quasi-self-adjointness. Although his arguments typically works only in finite-dimensional Hilbert spaces, the main idea is there: a $\mathcal{PT}$-symmetric operator is quantum mechanically relevant as a representative of a physical observable only if it is quasi-self-adjoint.

Once again, let us emphasise that, contrary to what one can occasionally read in physics papers, $\mathcal{PT}$-symmetric quantum mechanics is by no means any sort of extension of quantum mechanics. Anyway, the simple symmetry relation (1.5) provides a useful test which sometimes (but not always!) indeed guarantees that the spectrum of a non-self-adjoint operator H is real (*cf* Section 1.2.1). More importantly, $\mathcal{PT}$-symmetric quantum mechanics of Bender *et al.* has stimulated a new interest of various physical and mathematical communities in non-self-adjoint operators (including the author of the present thesis).

Apart from the conceptual applicability of quasi-self-adjoint $\mathcal{PT}$-symmetric operators in quantum mechanics, there has been a sudden availability of *experiments* with $\mathcal{PT}$-symmetry-like structures in *optics* [48, 58, 57, 4, 65]. This is due to the analogy of the time-dependent Schrödinger equation for a quantum particle subject to an external electromagnetic field and the paraxial approximation for a monochromatic light propagation in optical media. The physical significance of $\mathcal{PT}$-symmetry in this case is a balance between gain and loss [13]. At the same time, Schrödinger operators with complex potentials have been recently employed in experiments with *Bose-Einstein condensates*, where the imaginary part of the complex coupling models the injection and removal of particles [14].

1.2 Mathematical challenges

From the mathematical point of view, the theory of self-adjoint operators is well understood, while the non-self-adjoint theory is still in its infancy. Or maybe more appropriate would be to say that the theory is "under-developed". Indeed, according to the account given in [64, p. viii], the first pioneering works of G. D. Birkhoff from 1908–1913 [8, 9, 10] on non-self-adjoint boundary value problems were written almost at the same time as D. Hilbert's famous papers from 1904–1910 (*cf* [28]) that initiated self-adjoint spectral theory. But it was not until M. V. Keldyš' work from 1951 [32] when first abstract results on non-self-adjoint problems appeared in the literature, while the self-adjoint theory was already enjoying all the pleasures of life due to the needs of quantum mechanics at that time.

It is frustrating that the powerful techniques of the self-adjoint theory, such as the spectral theorem and variational principles, are not available for non-self-adjoint operators. Moreover, recent studies have revealed that this *lack of tools* is fundamental; the non-self-adjointness may lead to new and unexpected phenomena. Although there exist many interesting observations coming from physics and numerical studies of non-self-adjoint problems, the deep theoretical understanding is still missing and there is a need for new ideas and techniques.

The problem is that the non-self-adjoint theory is much more diverse and it is difficult, if not impossible, to find a common thread. *Indeed it can hardly be called a theory.* This is a quotation from the preface of E. B. Davies 2007 book [16], where a significant amount of work on spectral theory of non-self-adjoint operators can be found. He continues by the sentences on page ix that the present author has chosen as a motto of this thesis.

We particularly agree that the way how "to acquire the much wider range of knowledge" is by studying many distinct cases. This thesis is particularly concerned with various cases coming from the rapidly developing fields of quasi-Hermitian and $\mathcal{PT}$-symmetric quantum mechanics.

Let us now formulate a couple of specific mathematical problems related to non-self-adjoint operators.

1.2.1 Location of the spectrum

The spectrum of any self-adjoint operator is real and non-empty. On the other hand, there exist examples of non-self-adjoint operators for which the spectrum is the whole complex plane or empty. For instance, the spectrum of the *imaginary Airy oscillator*

$$-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + ix \qquad \text{in} \qquad L^2(\mathbb{R}) \tag{1.7}$$

considered on its maximal domain is easily seen to be empty (indeed, by the shift $x \mapsto x + c$ with $c \in \mathbb{C}$, the whole complex plane would must belong to the point spectrum, which however contradicts the fact that (1.7) is an operator with compact resolvent). In general, it turns out that even the very existence of *a* spectrum for a non-self-adjoint operator might be a highly non-trivial task (like for example for higher-dimensional versions of (1.7) on a half-space, subject to Dirichlet boundary condition [3]).

Even if ignoring the question of existence of a spectrum, how to locate the complex regions where the possible spectrum could exist? The minimax principle provides a powerful tool to estimate the location of discrete eigenvalues of a self-adjoint operator. Unfortunately, no variational replacement of this type is available in the non-self-adjoint case. It is true that the spectrum of any operator H satisfying some extra assumptions (such as m-sectoriality) is a subset of the *numerical range*

$$\mathsf{Num}(H) := \big\{ \langle \psi, H\psi \rangle : \ \psi \in \mathsf{D}(H)\,, \ \|\psi\| = 1 \big\}\,, \tag{1.8}$$

but such estimates are typically very rough and not useful in concrete examples. For instance, the spectrum of (1.7) is empty, while the numerical range coincides with the right complex half-plane. Summing up, providing good estimates on the spectrum of a non-self-adjoint operator is typically a hard task.

Why the spectrum of a non-self-adjoint $\mathcal{PT}$-symmetric operator might be expected to be located on the real line? A simple argument goes as follows. Let H_0 in $L^2(\mathbb{R}^d)$ be a self-adjoint operator with compact resolvent and assume that all the eigenvalues of H_0 are simple (a concrete example is the one-dimensional quantum harmonic oscillator). Consider a $\mathcal{PT}$-symmetric bounded potential $V : \mathbb{R}^d \to \mathbb{C}$ (*i.e.* $\overline{V(-x)} = V(x)$ for all $x \in \mathbb{R}^d$). It is easy to see that the symmetry (1.5) ensures that the eigenvalues of $H := H_0 + V$ are either real or come in complex-conjugate pairs. By standard perturbation theory, the perturbed eigenvalue of H remain simple, and therefore real, provided that $\|V\|$ is small. Furthermore, assuming some extra hypotheses (like for instance that the gaps between the eigenvalues of H_0 are bounded from below by a positive constant), it is even possible to ensure that the total spectrum of H is empty. Of course, such an argument is not applicable for the imaginary cubic oscillator (1.6), because the cubic potential is by no means a small perturbation of the

Laplacian. In general, it is difficult to prove that the spectrum of a $\mathcal{PT}$-symmetric operator is purely real, and in many examples it is not even true (in fact, it is generically not true [62]).

Many parts of this thesis are concerned with spectral analysis of non-self-adjoint differential operators, most of them being $\mathcal{PT}$-symmetric. We shall be particularly interested in the location of the essential spectrum and in establishing conditions which guarantee the existence or absence of eigenvalues.

1.2.2 Basis properties

The spectral theorem implies that the eigenvectors of a self-adjoint operator with compact resolvent can be chosen in such a way that they form an *orthonormal basis*. This useful property does not hold for non-self-adjoint operators. What is worse, the eigenvectors of a non-self-adjoint operator with compact resolvent might not be even *complete* in the sense that their span is not dense in the underlying Hilbert space (an obvious example is given by the imaginary Airy operator (1.7), for which there are no eigenfunctions). There are also examples of non-self-adjoint operators (some appear in the body of the thesis below) for which the eigenvectors form a complete set but not a *(Schauder) basis* in the sense that not every vector from the Hilbert space can be uniquely decomposed into the eigenvectors. Conditions guaranteeing that the eigenvectors (possibly together with the generalised eigenvectors) of non-self-adjoint operators form *a kind of* basis have been studied since the beginning of spectral theory (see [23] for an early survey), and it is also one of the interests of the present thesis.

In the context of quasi-Hermitian quantum mechanics, the natural requirement is that the normalised eigenvectors $\{\psi_j\}_j$ of a non-self-adjoint operator form at least a *Riesz basis* in the sense that they form the basis and there exists a positive constant C such that for every vector ψ of the Hilbert space the following inequalities hold

$$C^{-1}\|\psi\|^2 \leq \sum_j |\langle\psi_j,\psi\rangle|^2 \leq C\|\psi\|^2 \,. \tag{1.9}$$

Indeed, for an operator with compact resolvent and purely real eigenvalues, the eigenfunctions form a Riesz basis, if and only if, the operator is quasi-self-adjoint. Notice that eigenfunctions of a self-adjoint operator can be chosen in such a way that (1.9) is satisfied with $C = 1$ (Parseval's equality). Again, the literature on Riesz basis properties of non-self-adjoint operators is enormous (see [49] and references therein). Quasi-self-adjoint quantum mechanics has brought a new source of motivations, particularly for Schrödinger operators with complex potentials.

Let H be a quasi-self-adjoint operator with compact resolvent. Then its normalised eigenfunctions ψ_j form a Riesz basis. Denoting by ϕ_j the eigenfunctions of the adjoint H^* satisfying the biorthonormal relation $\langle\phi_j,\psi_k\rangle = \delta_{jk}$ for all j,k, it is easy to see that the metric operator Θ from (1.3) can be constructed according to the formula

$$\Theta = \sum_j c_j\,\phi_j\langle\phi_j,\cdot\rangle\,, \tag{1.10}$$

where c_j are positive numbers satisfying the inequalities $C^{-1} \leq c_j \leq C$ for all j with some positive constant C (independent of j). Different choices of c_j lead to different operators Θ, which reflects the well known non-uniqueness of the metric operator. In infinite-dimensional Hilbert spaces, one cannot expect to be able to sum up the series in (1.10), even if the eigenfunctions are known explicitly. One of the main contributions of this thesis is to provide models and techniques which make possible to turn (1.10) into a closed form.

1.2.3 Pseudospectra

The spectrum of any self-adjoint operator is stable in the sense that it is moved in the complex plane at most by the norm of the (possibly non-self-adjoint) perturbation. On the other hand, non-self-adjoint operators can be highly unstable in the sense that the spectrum of a small perturbation of a non-self-adjoint operator can be very far from the unperturbed spectrum. Given any positive number ε, let us quantify these *spectral instabilities* by introducing the notion of *ε-pseudospectra*

$$\sigma_\varepsilon(H) := \bigcup_{\|V\|<\varepsilon} \sigma(H+V)\,, \tag{1.11}$$

where H is a closed operator and V is an arbitrary bounded operator.

If H were self-adjoint, then the set $\sigma_\varepsilon(H)$ would be just the ε-tubular neighbourhood of the spectrum $\sigma(H)$. This follows from an equivalent characterisation of the pseudospectrum

$$\sigma_\varepsilon(H) = \sigma(H) \cup \left\{z\in\mathbb{C}\setminus\sigma(H):\ \|(H-z)^{-1}\| > \varepsilon\right\}$$

and the well known identity $\|(H-z)^{-1}\| = \operatorname{dist}(z,\sigma(H))^{-1}$ for self-adjoint (or more generally normal) operators. For general operators, however, one has only the inequality $\|(H-z)^{-1}\| \geq \operatorname{dist}(z,\sigma(H))^{-1}$ and therefore just the inclusion

$$\big\{z \in \mathbb{C} : \ \operatorname{dist}\big(z,\sigma(H)\big) < \varepsilon\big\} \subset \sigma_\varepsilon(H) \tag{1.12}$$

and there exist examples of non-self-adjoint operators for which the set on the right-hand side is much larger. The existence of large pseudospectra has in particular drastic consequences for numerical analysis of non-self-adjoint operators. We refer to by now classical monographs by L. N. Trefethen and M. Embree [63] and E. B. Davies [16] for more information on the notion and properties of pseudospectra and many references. The reader can also consult Appendix A.

One of the main objectives of this thesis is to advocate the usage of pseudospectra instead of spectra in quantum mechanics with non-self-adjoint operators. The main idea is that the quasi-self-adjointness of an operator ensures that its pseudospectrum cannot be too wild. More specifically, it is easy to see that if H is quasi-self-adjoint, then its pseudospectrum is *trivial* in the sense that there exists a constant C such that, for all positive ε,

$$\sigma_\varepsilon(H) \subset \big\{z \in \mathbb{C} : \ \operatorname{dist}\big(z,\sigma(H)\big) < C\varepsilon\big\} \,. \tag{1.13}$$

Notice that for a self-adjoint (or more generally normal) operator the inclusion (1.13) holds with $C = 1$. Hence, an operator is quantum-mechanically relevant as a representative of a physical observable only if its pseudospectrum is trivial. We shall see that the pseudospectra of many paradigmatic $\mathcal{PT}$-symmetric operators like (1.6) are highly non-trivial, and therefore quantum-mechanically irrelevant in this context.

Chapter 2

Presentation of results

This chapter is devoted to a brief and intentionally somewhat informal summary of the results presented in the subsequent chapters. The latter represent research articles of the author and are divided into the following three parts:

I. toy models,

II. waveguides,

III. pseudospectra.

This division may seem a bit artificial and there are indeed intersections. However, the individual papers were initially motivated by various objectives and this is reflected in different types of operators or results typically considered in the respective parts.

Part I is mainly motivated by the lack of rigorous approach to quasi-self-adjointness and unavailability of closed formulae for the metric operator (1.10) in the literature, at least at the time the presented papers appeared. The models presented in this part are typically Sturm-Liouville operators on a bounded interval with purely discrete spectrum.

On the other hand, Part II collects our papers on non-self-adjoint partial differential operators on unbounded domains (not necessarily tubes). Here the operators possess an essential spectrum and the main task is about the existence and location of possible eigenvalues.

Finally, Part III is motivated by our original observation that the paradigmatic models of $\mathcal{PT}$-symmetric quantum mechanics like (1.6) are not quasi-self-adjoint. For these results we advocate the mathematical notion of pseudospectrum as the right tool to rigorously describe the quasi-self-adjointness and other non-self-adjoint aspects of spectral theory. Here the considered operators are typically (but not exclusively) one-dimensional Schrödinger operators with complex potentials on an unbounded interval.

2.1 *Ad* Part I: Toy models

Shortly after the advent of $\mathcal{PT}$-symmetric quantum mechanics at the turn of the millennium, it was commonly accepted by the physics community that it is the quasi-self-adjointness which is behind the reality of the spectrum of non-self-adjoint $\mathcal{PT}$-symmetric operators like (1.6). There have been many sustained attempts to calculate the metric operator using formula (1.10) for various $\mathcal{PT}$-symmetric models of interest. Because of the complexity of the problem, however, it is not surprising that most of the available results were just approximative, usually expressed as leading terms of formal perturbation series. Moreover, there was a systematic lack of rigorous approach, leaving aside the domain issue of unbounded operators appearing in the series and making thus the results unjustified on a mathematically rigorous level. (In part III we shall see that this lack of rigorous approach is in fact fundamental and many of the paradigmatic $\mathcal{PT}$-symmetric models actually do not possess a regular metric.)

The state of the art at that time motivated the present author to enter the community and introduce a new model for which the metric operator and other related objects can be computed in a closed form (and in a rigorous way). The obtained results in this direction are presented in the following subsection. The other subsections contain our results on a model arising in a stochastic process and on non-self-adjoint graphs.

2.1.1 Complex Robin boundary conditions

The model and its quasi-self-adjointness

In the joint work [39] (Chapter 3) with H. Bíla and M. Znojil, we introduce the operator H_α in the Hilbert space $L^2\big((-a,a)\big)$ that acts as the Laplacian in the bounded interval $(-a,a)$ with $a>0$ and the only non-self-adjoint interaction comes from *complex boundary conditions* of Robin type:

$$H_\alpha\psi := -\psi'' \,, \qquad \psi \in \mathsf{D}(H_\alpha) := \big\{\psi \in W^{2,2}\big((-a,a)\big) : \ \psi' + i\alpha\psi = 0 \text{ at } \pm a\big\} \,, \tag{2.1}$$

where $\alpha \in \mathbb{R}$. Since $H_\alpha^* = H_{-\alpha}$, the operator H_α is not self-adjoint unless $\alpha = 0$, but it is $\mathcal{PT}$-symmetric in the sense of (1.5). The Sobolev space $W^{2,2}\big((-a,a)\big)$ consisting of functions that belong to $L^2\big((-a,a)\big)$ together with their first and second weak derivatives makes H_α well defined as an m-sectorial operator with compact resolvent. Consequently, the spectrum of H_α is composed of isolated eigenvalues of finite algebraic multiplicities located in a sector in the complex plane.

The eigenvalue problem $H_\alpha\psi = k^2\psi$ admits explicit solutions giving the spectrum

$$\sigma(H_\alpha) = \big\{k_n^2\big\}_{n=0}^\infty \qquad \text{with} \qquad k_j := \begin{cases} \alpha & \text{if} \quad n = 0\,, \\ \dfrac{n\pi}{2a} & \text{if} \quad n \geq 1\,. \end{cases} \tag{2.2}$$

The corresponding set of (unnormalised) eigenfunctions $\{\psi_n\}_{n=0}^\infty$ can be chosen as

$$\psi_n(x) := \cos\big(k_n(x+a)\big) - i\,\frac{\alpha}{k_n}\,\sin\big(k_n(x+a)\big)\,. \tag{2.3}$$

Surprisingly, the spectrum of H_α is purely real. However, notice that if $\alpha \in k_1\,\mathbb{Z}\setminus\{0\}$, then H_α admits an eigenvalue of geometric multiplicity one and algebraic multiplicity two (a Jordan block); in this case H_α cannot be similar to a self-adjoint operator. Apart from these exceptional values of α, it is shown in [39] that H_α is quasi-self-adjoint. Moreover, using (1.10) and the explicit form of the eigenfunctions (2.3), a closed formula for the metric Θ satisfying the quasi-self-adjointness relation (1.3) is found.

We are honoured that our model (2.1) was included by B. Helffer in his new book, *cf* [24, Ex. 13.5].

Alternative formulae for the metric and more

In [36] (Chapter 4), an alternative form for the metric is found with help of a *backward use of the spectral theorem*. This new idea is inspired by the observation that the eigenfunctions (2.3) for $n \geq 1$ are a sum of eigenfunctions of the (self-adjoint) Dirichlet and Neumann Laplacians in $L^2\big((-a,a)\big)$. In this way, the metric operator Θ of [36] is expressed in terms of resolvents of these operators.

In the joint work [46] (Chapter 5) with P. Siegl and J. Železný (author's student), using a special normalisation of (2.3) and explicit formulae for the resolvents of the Dirichlet and Neumann Laplacians, we obtain a particularly simple formula for the metric operator

$$\Theta = I + K \qquad \text{with} \qquad \mathcal{K}(x,y) := \alpha\, e^{-i\alpha(y-x)}\,\big[\tan(\alpha a) - i\,\mathrm{sgn}(y-x)\big]\,, \tag{2.4}$$

where $\mathcal{K}$ denotes the integral kernel of K. Furthermore, we eventually manage to find a *self-adjoint* operator

$$h_\alpha\psi := -\psi'' + \alpha^2\,\chi_0^N\langle\chi_0^N,\cdot\rangle\,, \qquad \psi \in \mathsf{D}(h_\alpha) := \big\{\psi \in W^{2,2}\big((-a,a)\big) : \ \psi' = 0 \text{ at } \pm a\big\}\,, \tag{2.5}$$

to which H_α is similar in the sense of (1.4) (with a metric $\Theta = \Omega^*\Omega$ different to (2.4)), where $\chi_0^N(x) := 1/\sqrt{2a}$ is the first eigenfunction of the Neumann Laplacian in $(-a,a)$. Since h_α is just a rank-one perturbation of the Neumann Laplacian, the spectral picture (2.2) is clearly explained.

In fact, in [46], we proceed in a much greater generality by allowing α in (2.1) to be complex and achieving possibly different values at $\pm a$ (leading thus to a not necessarily $\mathcal{PT}$-symmetric model). General properties of the similarity transforms to self-adjoint and normal operators are studied in detail.

Physical interpretations

Notice that the self-adjoint counterpart h_α of H_α given in (2.5) has the form of the *Friedrichs Hamiltonian*, which has been used in various circumstances in quantum mechanics, *cf* [30]. In this way, our work [46] provides a potential interpretation of the model (2.1) as an unconventionally represented quantum Hamiltonian.

In the joint work [27] (Chapter 6) with H. Hernandez-Coronado and P. Siegl, we propose another quantum-mechanical interpretation of the model (2.1), this time directly in terms of a *perfect-transmission scattering*.

The idea is that the one-dimensional scattering problem $-\psi'' + V\psi = k^2\psi$ on the whole real line in the regime of perfect transmission, where k is a positive (wave) number and the scattering potential $V : \mathbb{R} \to \mathbb{R}$ is bounded and supported in $[-a, a]$, leads to the non-linear problem

$$\begin{cases} -\psi'' + V\psi = k^2\psi & \text{in} \quad [-a, a]\,, \\ \psi' - ik\psi = 0 & \text{at} \quad \pm\, a\,. \end{cases}$$

This operator-pencil problem (the boundary condition depends on energy) can be solved by considering the associated one-parametric (linear) spectral problem

$$\begin{cases} -\psi'' + V\psi = \mu\psi & \text{in} \quad [-a, a]\,, \\ \psi' - i\alpha\psi = 0 & \text{at} \quad \pm\, a\,, \end{cases} \tag{2.6}$$

where $\mu = \mu(\alpha)$ plays the role of eigenvalue and α is a real parameter. Indeed, the energies corresponding to the perfect-transmission states are found as those points satisfying

$$\mu(\alpha) = \alpha^2\,.$$

Clearly, (2.6) is just the eigenvalue problem for $H_{-\alpha} + V$ with H_α being our toy model from (2.1).

Finally, let us mention that the boundary conditions employed in our model (2.1) are known as *impedance* boundary conditions in electromagnetism. In a quantum-mechanical context, they have been used previously by H.-Ch. Kaiser, H. Neidhardt and J. Rehberg in [31] to model open systems in semiconductor physics. In their setting, the parameter $i\alpha$ is allowed to be complex but its imaginary part has opposite signs on the boundary points such that the system is dissipative. In our case (2.1), we actually deal with *radiation/absorption* boundary conditions in the language of theory of electromagnetic field and the $\mathcal{PT}$-symmetry is reflected in the *gain/loss balance*. Related scattering experiments in optics were performed in [4].

Curved spaces

In the joint work [42] (Chapter 7) with P. Siegl, we consider the Laplace-Beltrami operator in tubular neighborhoods of curves on two-dimensional Riemannian manifolds, subject to complex Robin-type boundary conditions. We focus on manifolds of constant curvature, *cf* Figure 7.2, when the spectral problem reduces to the study of Sturm-Liouville operators in $L^2\big((-a, a)\big)$, subject to boundary conditions of the type of (2.1).

For zero curvature, we recover the pure Laplacian case (2.1). If the curvature is positive, it turns out that the spectrum is purely real. More precisely, it is proved only for higher eigenvalues, but our numerical simulations suggest that it is always the case. For negative curvature, we prove that there are also complex-conjugate eigenvalues. In any case, if the spectrum is simple, it follows that the Sturm-Liouville operator is similar to a self-adjoint or at least normal operator.

The Pauli equation

In the joint work [33] (Chapter 8) with D. Kochan, R. Novák (author's student) and P. Siegl, we extend the model (2.1) to operator matrices

$$\begin{pmatrix} -\dfrac{\mathrm{d}^2}{\mathrm{d}x^2} + b & 0 \\ 0 & -\dfrac{\mathrm{d}^2}{\mathrm{d}x^2} - b \end{pmatrix} \qquad \text{in} \qquad L^2\big((-a, a); \mathbb{C}^2\big)\,,$$

subject to general boundary conditions

$$\psi'(\pm a) + A^{\pm}\psi(\pm a) = 0\,,$$

where b is a real parameter (magnetic field) and the matrices $A^{\pm} \in \mathbb{C}^{2\times 2}$ model a possibly non-self-adjoint interaction. We are again concerned with spectral properties and with the question of quasi-self-adjointness. A remarkable property of this model is that the time-reversal operator $\mathcal{T}$ differs from the complex conjugation and satisfies $\mathcal{T}^2 = -I$ (as usual for fermionic systems).

2.1.2 Stochastic physics meets quantum mechanics

In the joint work [34] (Chapter 9) with M. Kolb, we apply the ideas of quasi-self-adjoint quantum mechanics to give an insight into peculiar properties of a stochastic process. Consider a Brownian particle with a constant quadratic variation in the bounded interval $(-\frac{\pi}{2}, \frac{\pi}{2})$ and wait until it hits one of the boundary points $\pm\frac{\pi}{2}$. At the hitting time, the Brownian particle gets restarted in an interior point $\frac{\pi}{2}a$ with $a \in (-1, 1)$ and repeats the process at the previous step. The generator of this process can be described by the non-self-adjoint operator

$$H\psi := -\psi'' , \qquad \psi \in \mathsf{D}(H) := \left\{\psi \in W^{2,2}((-\tfrac{\pi}{2}, \tfrac{\pi}{2})) : \ \psi(-\tfrac{\pi}{2}) = \psi(\tfrac{\pi}{2}a) = \psi(\tfrac{\pi}{2})\right\} , \tag{2.7}$$

in the Hilbert space $L^2\big((-\frac{\pi}{2}, \frac{\pi}{2})\big)$.

It has been known to probabilists (including my co-author) that the eigenvalues of this operator are purely real and that the spectral gap coincides with the second eigenvalue of the Dirichlet Laplacian in $L^2\big((-\frac{\pi}{2}, \frac{\pi}{2})\big)$ (this is also true for more general models, *cf* [5]). In fact, the eigenvalue problem for (2.7) can be solved explicitly. What is the mechanism behind these properties?

In our paper [34], we prove that H is an m-accretive operator with compact resolvent, so that the *total* spectrum of H is indeed purely real (for it is composed of eigenvalues only). The main idea is to compute the adjoint H^*, which also enables us to determine the geometric and algebraic multiplicities of the eigenvalues. It turns out that spectral characteristics of H depends on *Diophantine properties* of a. If a is irrational, then all eigenvalues are algebraically simple. If a is rational, then there exist eigenvalues of geometric multiplicity two and algebraic multiplicity three (Jordan blocks).

In either case, the eigenfunction of H do not form a basis (not even Schauder's, though the eigenfunctions are always minimally complete if a is irrational). Consequently, the quasi-self-adjointness relation (1.3) cannot hold with bounded and boundedly invertible Θ. If a is irrational, however, we show that the *weaker* relation

$$H^*\Theta = \Theta H \tag{2.8}$$

does hold with a bounded positive operator Θ (which is not necessarily boundedly invertible). Consequently, H is "quasi-self-adjoint" in a generalised sense. Moreover, using the special form of eigenfunctions of the adjoint H^*, we provide a spectacularly simple formula for the metric operator

$$\Theta = \phi_0\langle\phi_0, \cdot\rangle + P_0 + P_- \oplus P_+ .$$

Here ϕ_0 is an eigenfunction of H^* corresponding to the zero eigenvalue, P_0 is the antisymmetric projection with respect to the middle point 0 of $(-\frac{\pi}{2}, \frac{\pi}{2})$, the direct sum is with respect to the decomposition $L^2\big((-\frac{\pi}{2}, \frac{\pi}{2})\big) = L^2\big((-\frac{\pi}{2}, \frac{\pi}{2}a)\big) \oplus L^2\big((\frac{\pi}{2}a, \frac{\pi}{2})\big)$, P_- is the antisymmetric projection with respect to the middle point $-\frac{\pi}{4}(1-a)$ of $(-\frac{\pi}{2}, \frac{\pi}{2}a)$ and P_+ is the antisymmetric projection with respect to the middle point $\frac{\pi}{4}(1+a)$ of $(\frac{\pi}{2}a, \frac{\pi}{2})$.

2.1.3 Non-self-adjoint graphs

In the joint work [29] (Chapter 10) with A. Hussein and P. Siegl, motivated by the growing interest in network models and in quasi-self-adjoint quantum mechanics, we consider the Laplacian on metric graphs, subject to general (possibly non-self-adjoint) interface or boundary conditions on the graph vertices. We regard the graphs as an intermediate step between Sturm-Liouville operators on intervals and partial differential operators, moving naturally from the one-dimensional toy models of Part I to higher-dimensional structures of Part II.

The Hilbert space of a metric graph Γ is the direct sum

$$L^2(\Gamma) := \bigoplus_{j=1}^{N} L^2\big((0, a_j)\big) ,$$

where N is a natural number denoting the number of graph *edges* $(0, a_j)$, where each *length* a_j is either a positive number or infinity. The natural number

$$d := \#(\text{unbounded edges}) + 2\,\#(\text{bounded edges})$$

is called the *dimension* of the graph. On this Hilbert space, we consider the operator

$$H\psi := -\psi'' , \qquad \psi \in \mathsf{D}(H) := \left\{\psi \in W^{2,2}(\Gamma) : \ A\underline{\psi} + B\underline{\psi}' = 0\right\} ,$$

where $\underline{\psi}$ is a d-dimensional vector composed of boundary values of ψ and $A, B \in \mathbb{C}^{d\times d}$ are arbitrary matrices. The operator H is self-adjoint if, and only if, $AB^* = BA^*$, and this case is well studied in the literature due to applications in quantum nanostructures (see references given in Chapter 10). On the other hand, in [29] we are primarily interested in non-self-adjoint graph realisations, which is essentially an unexplored area.

There are several objectives of our paper [29]. First of all, we propose a *new classification* of the boundary conditions, calling the graph *regular* if $A + ikB$ is invertible for some $k \in \mathbb{C}$, and *irregular* otherwise. That this classification is indeed useful is illustrated on many *examples* of regular and irregular graphs. The spectrum of irregular graphs is typically quite singular: either empty or covering the whole complex plane. On the other hand, we show that the spectrum of regular graphs is neither empty nor the whole complex plane and establish some general *spectral properties* about the point, residual and essential spectra. For instance, the closure of the point spectrum is a discrete set and the residual spectrum exists only for graphs with both bounded and unbounded edges, and in this case it is a discrete subset of the essential spectrum $[0, \infty)$. On compact graphs, we investigate the existence of a *Riesz basis* of projectors and similarity transforms to self-adjoint Laplacians.

The most interesting result of [29] is probably the following simple way how to relate the similarity transforms between Laplacians on certain graphs with elementary similarity transforms between the matrices defining the boundary conditions. For graphs with bounded edges of the same length, we show that if $A' = G^{-1}AG$ and $B' = G^{-1}BG$ with an invertible matrix $G : \mathbb{C}^d \to \mathbb{C}^d$, then there exists a bounded and boundedly invertible transform $\Omega_G : L^2(\Gamma) \to L^2(\Gamma)$ such that (*cf* (1.4))

$$H' = \Omega_G^{-1} H \Omega_G \,,$$

where H' is defined as H but with A', B' instead of A, B. In particular, if H' is self-adjoint (*i.e.*, $A'B'^* = B'A'^*$), then H is quasi-self-adjoint.

2.2 *Ad* Part II: Waveguides

In this part we collect author's papers on non-self-adjoint partial differential operators. Chapters 11–15 are concerned with "genuine waveguides" in the sense of a tubular geometry, while Chapters 16, 17 and 18 are included mainly because of the similarity with waveguides via the presence of an essential spectrum.

2.2.1 Complex Robin boundary conditions

The model and discrete real eigenvalues

In the joint work [11] (Chapter 11) with D. Borisov, we extend the toy model (2.1) to higher dimensions by considering the two-dimensional operator

$$H_\alpha \psi := -\Delta\psi \,, \qquad \psi \in \mathsf{D}(H_\alpha) := \big\{\psi \in W^{2,2}\big(\mathbb{R} \times (-a,a)\big) : \ \partial_2\psi + i\alpha\psi = 0 \text{ on } \mathbb{R} \times \{\pm a\}\big\} \,, \tag{2.9}$$

where $\alpha : \mathbb{R} \to \mathbb{R}$ is a Lipschitz function. Again, since $H_\alpha^* = H_{-\alpha}$, the operator is not self-adjoint unless $\alpha = 0$, but it is a well-defined m-sectorial operator in $L^2\big(\mathbb{R} \times (-a,a)\big)$, which is $\mathcal{PT}$-symmetric with respect to $(\mathcal{P}\psi)(x_1, x_2) := \psi(x_1, -x_2)$ and $(\mathcal{T}\psi)(x) := \overline{\psi(x)}$. In [11] we additionally remark that H_α is $\mathcal{T}$-self-adjoint in the sense that $H_\alpha^* = \mathcal{T}H_\alpha\mathcal{T}$, which generally implies that the residual spectrum of H_α is empty.

Assuming that the boundary conditions are *homogeneous* in the sense that $\alpha(x_1) = \alpha_0 \in \mathbb{R}$ for all $x_1 \in \mathbb{R}$, we show that the spectrum of H_{α_0} is purely real and essential,

$$\sigma(H_{\alpha_0}) = \sigma_{\mathrm{ess}}(H_{\alpha_0}) = [\mu_0^2, \infty) \qquad \text{with} \qquad \mu_0^2 := \min\left\{\alpha_0^2, \left(\frac{\pi}{2a}\right)^2\right\} .$$

In [11] we are interested in *local perturbations* of H_{α_0}. Assuming that $\alpha(x)$ tends to a constant α_0 as $|x| \to \infty$, we show that the essential spectrum of H_α coincides with the spectrum of H_{α_0}. Our main interest is in the existence of *discrete eigenvalues*. Writing $\alpha(x_1) = \alpha_0 + \varepsilon\beta(x_1)$ with $\beta \in C_0^2(\mathbb{R})$ and positive ε, we show that H_α has no eigenvalues converging to μ_0^2 as $\varepsilon \to 0$ provided that $\alpha_0 = 0$ or $\alpha_0 \int_{\mathbb{R}} \beta > 0$. On the other hand, if $\alpha_0 \int_{\mathbb{R}} \beta < 0$, we show that H_α possesses a simple (and therefore real) eigenvalue λ_ε satisfying the asymptotic formula

$$\lambda_\varepsilon = \mu_0^2 - \varepsilon^2\, \alpha_0^2\, (\textstyle\int_{\mathbb{R}} \beta)^2 + O(\varepsilon^3) \qquad \text{as} \qquad \varepsilon \to 0 \,. \tag{2.10}$$

We also establish existence/absence results in the critical case $\int_{\mathbb{R}} \beta = 0$ and, if the eigenvalue exists, we improve the asymptotic formula by finding the term of order ε^3 as well.

The approach of [11] to the discrete spectrum of H_α is based on the method of matched asymptotic expansions. Author's student R. Novák later established similar results (also for a three-dimensional waveguide) by the Birman-Schwinger method [55]. The latter enables one to relax the regularity hypothesis about β, but only the low-order asymptotics (2.10) is found.

Numerical analysis and non-real eigenvalues

The asymptotic study of [11] leaves open the question whether the model (2.9) may possess non-real eigenvalues as well. To this purpose, in the joint work [47] (Chapter 12) with M. Tater, we investigate the existence/absence of eigenvalues of H_α by numerical methods. In addition to obtaining a good agreement with the asymptotic formula (2.10), we identify regimes of α_0 and β for which there exist complex-conjugate pairs of eigenvalues together with real spectra. We particularly invite the reader to watch the animation on author's homepage:

`http://gemma.ujf.cas.cz/~krejcirik/KT.html`

Open problems

Based on the study performed in [11] and [47] as well as on the previous experience of the author with self-adjoint waveguides, in the short invited note [38] (Chapter 13), we point out the need for a robust method establishing the existence of eigenvalues for non-self-adjoint operators possessing an essential spectrum. Another open problem is about the absence of eigenvalues for non-self-adjoint operators (*cf* Chapter 17).

Thin waveguides and other results

In the joint work [12] (Chapter 14) with D. Borisov, we study the operator (2.9) in the limit when the width of the waveguides tends to zero. More specifically, we establish the operator convergence

$$H_\alpha \xrightarrow[a\to 0]{} -\frac{\mathrm{d}^2}{\mathrm{d}x_1^2} + \alpha(x_1)^2 \tag{2.11}$$

in a norm-resolvent sense. Since the operator on the right-hand side is self-adjoint, we obtain a heuristic support for the existence of real spectra of H_α. Moreover, the eigenvalue asymptotics of the self-adjoint operator coincides with (2.10). The results of [12] are more general in the sense that we consider the limit for an analogue of the model (2.9) in the layer $\mathbb{R}^{d-1} \times (-a, a)$ of arbitrary dimension $d \geq 2$.

In the joint work [41] (Chapter 15) with N. Raymond, J. Royer and P. Siegl, we extend the convergence result (2.11) to the case of the Laplacian $-\Delta_\alpha^{\Omega_a}$ in an a-tubular neighbourhood of an *arbitrary hypersurface* Σ in $\mathbb{R}^d$, subject to *more general Robin boundary conditions.* For illustration, restricting the very general result of [41] to the two-dimensional case of Σ being a curve and keeping the boundary conditions as in (2.9), we can write

$$-\Delta_\alpha^{\Omega_a} \xrightarrow[a\to 0]{} -\frac{\mathrm{d}^2}{\mathrm{d}s^2} + \alpha(s)^2 - i\,\alpha(s)\,\kappa(s) \tag{2.12}$$

in a norm-resolvent sense, where κ and s is the curvature and arc-length of Σ, respectively. Comparing (2.12) with (2.11), we clearly see the role of curvature on spectral properties of $-\Delta_\alpha^{\Omega_a}$ as $a \to 0$.

Let us emphasise that the objectives and results of [41] are much more universal than presented here. We actually provide an abstract approach for obtaining dimensional reductions via the norm-resolvent convergence. Our applications to the semiclassical Born-Oppenheimer approximation, shrinking tubular neighborhoods of hypersurfaces, *etc*, are just illustrative examples of the general scheme.

2.2.2 Singular interactions

In the joint work [35] (Chapter 16) with S. Kondej, we consider the operator formally written as

$$H_\varepsilon := -\Delta + \alpha_+\,\delta_{\Sigma_{+\varepsilon}} + \alpha_-\,\delta_{\Sigma_{-\varepsilon}} \qquad \text{in} \qquad L^2(\mathbb{R}^d)\,, \tag{2.13}$$

where $\alpha_\pm$ are two complex numbers and $\Sigma_{\pm\varepsilon} := \{q \pm \varepsilon n(q) : q \in \Sigma_0\}$ are parallel surfaces at the distance ε of the boundary $\Sigma_0 := \partial\Omega$ of a smooth bounded open set $\Omega \subset \mathbb{R}^d$, $d \geq 1$, with $n : \Sigma_0 \to \mathbb{R}^d$ denoting the outer unit normal to Ω. It is standard to give a rigorous meaning to the Schrödinger operator with Dirac interactions of the type (2.13) as an m-sectorial operator associated with a closed quadratic form. In this way, (2.13) can be considered as an extension of a curved variant of (2.9) to the whole space (in all dimensions). Contrary to (2.9), the singular interaction of (2.13) may achieve different values on $\Sigma_{\pm\varepsilon}$, but it is assumed to be constant on each of the parallel surfaces. The operator H_ε is non-self-adjoint unless the constants $\alpha_\pm$ are real.

It is natural to expect that H_ε will converge, in a certain sense, to the operator

$$H_0 := -\Delta + (\alpha_+ + \alpha_-)\,\delta_{\Sigma_0} \qquad \text{in} \qquad L^2(\mathbb{R}^d)\,.$$

The purpose of the paper [35] is to show that the convergence holds in the norm-resolvent sense and to establish asymptotic expansions for semisimple discrete eigenvalues of H_ε as $\varepsilon \to 0$. We stress that, because of the singular dependence of H_ε on ε, the eigenvalue asymptotics is not a consequence of analytic perturbation theory and a non-trivial rigorous approach is needed to reveal a geometric term in the asymptotic formula.

In the self-adjoint case, the results of [35] quantify the effect of tunnelling in coalescing heterostructures.

2.2.3 Absence of eigenvalues

In the joint work [20] (Chapter 17) with L. Fanelli and L. Vega, we consider electromagnetic Schrödinger operators

$$H_{A,V} := (-i\nabla + A)^2 + V \qquad \text{in} \qquad L^2(\mathbb{R}^d)\,, \tag{2.14}$$

where $A : \mathbb{R}^d \to \mathbb{R}^d$ is the magnetic (vector) potential and $V : \mathbb{R}^d \to \mathbb{C}$ is the electric (scalar) potential. In recent years, there have been an enormous increase of interest in Schrödinger operators with complex potentials, particularly motivated by the attempts to extend the Lieb-Thirring inequalities for the eigenvalues to the non-self-adjoint case (see references in Chapter 17). The main objective of [20] is to provide sufficient conditions which guarantee the *absence of eigenvalues* of $H_{A,V}$, including eigenvalues embedded in the continuous spectrum.

The first result of [20] is based on the *Birman-Schwinger principle* and it shows that the smallness form-subordinated condition

$$\exists a < 1\,, \quad \forall \psi \in W^{1,2}(\mathbb{R}^3)\,, \qquad \int_{\mathbb{R}^3} |V||\psi|^2 \leq a \int_{\mathbb{R}^3} |\nabla\psi|^2 \tag{2.15}$$

implies that the spectrum of the purely electric operator $H_{0,V}$ in three dimensions coincides with the spectrum of the free Hamiltonian,

$$\sigma(H_{0,V}) = \sigma_{\mathrm{c}}(H_{0,V}) = [0,\infty)\,. \tag{2.16}$$

In particular, the point and residual spectra of $H_{0,V}$ are empty. Condition (2.15) is an improvement upon existing results in the literature (*cf* [21]), in particular potentials with *critical singularities* satisfying $|V(x)| \leq a/(4|x|^2)$ can be included. It is also an improvement upon an analogous result in the self-adjoint case stated in terms of Rollnik-class potentials (*cf* [56, Thm. XIII.21]). We leave as an open problem whether the d-dimensional version of (2.15) is sufficient to conclude with (2.16) for every $d \geq 3$.

The other sufficient conditions of [20] are based on the *method of multipliers* and they imply the absence of eigenvalues of the operator $H_{A,V}$ in all dimensions $d \geq 3$ and possibly under the presence of magnetic field. By this method, we have not been able to fully reach condition (2.15). On the other hand, some of the alternative hypotheses are not "smallness", but rather sort of "repulsiveness" conditions. Let us also stress that the conditions on the magnetic field are stated in a gauge-invariant form.

2.2.4 Non-accretive Schrödinger operators and Agmon-type estimates

In the joint work [40] (Chapter 18) with N. Raymond, J. Royer and P. Siegl, we also consider the electromagnetic operator $H_{A,V}$ from (2.14), but now it can be restricted to a subdomain $\Omega \subset \mathbb{R}^d$, subject to Dirichlet boundary conditions.

Our main interest is to provide a closed realisation of $H_{A,V}$ with non-empty resolvent set in *non-accretive* situations, *i.e.* when the numerical range of the operator is not contained in a complex half-plane. It typically happens if the real part of V is not bounded from below. An illustrative example is given by the operator

$$-\frac{\mathrm{d}^2}{\mathrm{d}x^2} - x^2 + ix^3 \qquad \text{in} \qquad L^2(\mathbb{R})\,, \tag{2.17}$$

for which the numerical range covers the whole complex plane. In [40], we are able to give a meaning to (2.17) and even to potentials with a much wilder growth at infinity and/or oscillations.

Our approach is based on the generalised Lax-Milgram-type theorem of Y. Almog and B. Helffer [2] involving a new idea of *weighted coercivity*. We essentially require that the potentials are smooth and

$$|\nabla V(x)| + |\nabla B(x)| = o\Big(\big(|V(x)| + |B(x)|\big)^{3/2} + 1\Big)\,,$$
$$(\Re V(x))_- = o\Big(|V(x)| + |B(x)| + 1\Big),$$

as $|x| \to \infty$, where $(\Re V)_-$ is the negative part of $\Re V$ and $B := \mathrm{d}A$ is the magnetic tensor. Notice that $(\Re V)_-$ can be compensated not only by $\Im V$, but also by the magnetic field. Again, we stress that our conditions on the electromagnetic potentials are stated in a gauge-invariant form.

The ultimate goal of the paper [40] is to show that any eigenfunction ψ corresponding to a discrete eigenvalue λ satisfies the *Agmon-type exponential decay*

$$e^{\frac{1-\varepsilon}{3}\,\mathrm{d}_{\mathrm{Ag}}(x)}\,\psi \in L^2(\Omega)\,,$$

where $\varepsilon \in (0,1)$ is arbitrary and d_{Ag} is the *Agmon distance* satisfying

$$|\nabla \mathrm{d}_{\mathrm{Ag}}(x)|^2 = \big(\gamma_1|V(x)| - \Re\lambda - |\Im\lambda| - \gamma_2\big)_+$$

with suitable constants $\gamma_1 > 0$ and $\gamma_2 \in \mathbb{R}$. For (2.17) the result yields $e^{\delta|x|^{5/2}}\psi \in L^2(\mathbb{R})$ with some positive δ.

2.3 *Ad* Part III: Pseudospectra

Now we probably turn to the most significant results of the author. The next papers to be presented are interlinked by the appearance of the mathematical notion of pseudospectra.

2.3.1 The semiclassical fall of $\mathcal{PT}$-symmetric quantum mechanics

On the metric of the imaginary cubic oscillator

The imaginary cubic oscillator (1.6) can be considered as the *fons et origo* of $\mathcal{PT}$-symmetric quantum mechanics whose origin can be dated to 1998 [6]. The problem of similarity of the operator (1.6) to a self-adjoint operator was investigated in several works, see, *e.g.*, [7, 53]. However, due to the complexity of the task, the approach used in these papers was necessarily formal, based on developing the metric into an infinite series composed of unbounded operators. There existed no proof of quasi-self-adjointness of the imaginary cubic oscillator as late as 2012, when an important meeting of the $\mathcal{PT}$-symmetry community took part in Paris [66]. The reason was very simple: (1.6) is *not quasi-self-adjoint*, at least not in the sense of (1.3). This property was established in the joint work [61] (Chapter 19) with P. Siegl. More specifically, denoting by H the maximal (m-accretive) realisation of (1.6),

$$(H\psi)(x) := -\psi''(x) + ix^3\psi(x)\,, \qquad \psi \in \mathsf{D}(H) := \{\psi \in L^2(\mathbb{R}) :\ H\psi \in L^2(\mathbb{R})\}\,, \tag{2.18}$$

we prove the following important facts about (1.6):

1. *There exists a bounded metric.* More precisely, there exists a positive bounded operator Θ such that the weaker quasi-self-adjointness relation (2.8) holds.
2. *The metric is necessarily singular.* That is, no bounded metric operator Θ with bounded inverse satisfying (2.8) exists.

Mathematically, the first (positive) property is a consequence of the *completeness of eigenfunctions* of H that we prove as a new result in [61]. The second (negative) property means that the eigenfunctions *do not form a Riesz basis.* We conclude that the paradigmatic example (1.6) is not relevant as a representative of a physical observable in quantum mechanics.

The original idea of [61] to establish the absence of bounded and boundedly invertible similarity transformation of H to a self-adjoint operator is based on the concept of pseudospectra. More specifically, we show that the pseudospectrum of H is not trivial in the sense that the inclusion (1.13) is violated. By contradiction, let us assume that the pseudospectrum of H is trivial. Performing the scaling $(U_\hbar\psi)(x) := \hbar^{-1/5}\psi(\hbar^{-2/5}x)$ with any positive number $\hbar$, we cast H into a *semiclassical* operator

$$U_\hbar H U_\hbar^{-1} = \hbar^{-6/5}\, H_\hbar\,, \qquad \text{where} \qquad H_\hbar := -\hbar^2\frac{\mathrm{d}^2}{\mathrm{d}x^2} + ix^3\,.$$

Then, for any fixed $z \in \mathbb{C}$ with $\Re z > 0$ and $\Im z \neq 0$, we have

$$\frac{C}{\hbar^{-6/5}|\Im z|} \geq \frac{C}{\operatorname{dist}\big(\hbar^{-6/5}z, \sigma(H)\big)} > \|(H - \hbar^{-6/5}z)^{-1}\| = \hbar^{6/5}\,\|(H_\hbar - z)^{-1}\| \geq c_n\,\hbar^{-n}\,,$$

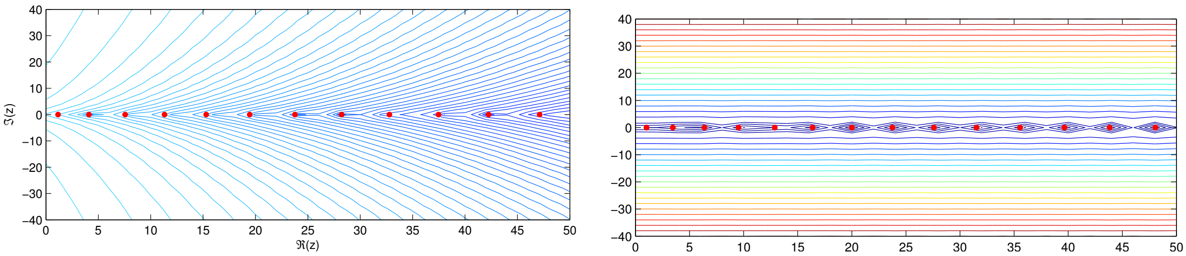
where the first inequality follows from the fact that the spectrum of H is real, the second inequality is due to the assumption that the pseudospectrum of H is trivial, the equality employs the scaling above and the last inequality (the crucial step) follows from known semiclassical results for non-self-adjoint Schrödinger operators that ensure that the resolvent of $H_\hbar$ diverges faster than any power of $\hbar^{-1}$ as $\hbar \to 0$. More specifically, it follows from E. B. Davies' result [15] that there exists a positive $\hbar_0$ and for each positive n a positive constant c_n such that, for all $\hbar \in (0, \hbar_0)$, the last inequality holds. Comparing the extreme left- and right-hand sides of the chain of inequalities above, we get a contradiction for all sufficiently small $\hbar$. Therefore the spectrum of H cannot be trivial.

Let us finally mention that our result from [61] about the absence of Riesz basis for (2.18) was later improved by R. Henry [25] who showed that the eigenfunctions do not even form a (Schauder) basis. The proof that the pseudospectrum of the modified model with a harmonic potential added to the imaginary cubic term is non-trivial was given by author's student R. Novák [54].

Transition from spectra to pseudospectra

The paper [61] was a brief account for the physics community in which we focus on the paradigmatic example (1.6). However, the methods of the paper, namely the disproval of quasi-self-adjointness based on the semiclassical pseudospectra, does not restrict to the particular model. Moreover, the pseudospectra instead of spectra universally seems to be the right concept to describe the subtleties of quantum mechanics with non-self-adjoint operators. This was our motivation to follow [61] with the joint work [45] (Chapter 20) with P. Siegl, M. Tater and J. Viola, in which we make a sort of overview of the notion of pseudospectra in the context of quasi-self-adjoint quantum mechanics. The abstract results are illustrated on many concrete examples familiar from $\mathcal{PT}$-symmetric quantum mechanics and elsewhere. We also perform a numerical analysis of the models.

To briefly summarise the usefulness of the concept of pseudospectra as advocated in [45], let us have a look at Figure 2.1. On the left picture, there is a numerically computed pseudospectrum of the imaginary cubic oscillator (2.18). The blue curves correspond to the level lines $\|(H-z)^{-1}\| = \varepsilon^{-1}$ in the complex z-plane for different small values of ε. We clearly see that the pseudospectrum can be located very far from the spectrum (the red dots corresponding to the real eigenvalues), resulting therefore in spectral instabilities due to (1.11) in accordance with our semiclassical analysis above. The pseudospectrum is thus obviously non-trivial and already this simple numerical check suggests that the operator cannot be quasi-self-adjoint. On the other hand, the right picture depicts numerically computed pseudospectra for a self-adjoint analogue of (2.18) and we clearly see that the ε-pseudospectrum is just the ε-tubular neighbourhood of the spectrum. For a quasi-self-adjoint operator, the pseudospectrum should be located at least in a tubular neighbourhood of the spectrum, *cf* (1.13).



$$-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + ix^3 \qquad\qquad -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + |x|^3$$

Figure 2.1: Pseudospectra of cubic oscillators. *(Courtesy of Miloš Tater.)*

One of the main new results obtained in [45] is the proof of a non-trivial pseudospectrum for the *imaginary shifted harmonic oscillator*

$$-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + (x+i)^2 \qquad \text{in} \qquad L^2(\mathbb{R}) \tag{2.19}$$

considered on its maximal domain. Notice that the scaling as above does not help, because the imaginary part of the potential is a small perturbation of the real part, so the known results about the semiclassical pseudospectrum do not apply here. Nevertheless, the desired result can be obtained by a standard construction of semiclassical pseudomodes even in this case.

2.3.2 The imaginary sign potential

In the joint work [26] (Chapter 21) with R. Henry, we introduce a new non-self-adjoint $\mathcal{PT}$-symmetric model

$$H := -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + i\,\mathrm{sgn}(x) \qquad \text{in} \qquad L^2(\mathbb{R}) \tag{2.20}$$

with natural domain $\mathsf{D}(H) := W^{2,2}(\mathbb{R})$. Our main motivation to consider this operator is the fact that it cannot be cast to a semi-classical operator. Moreover, the known techniques to study the semiclassical pseudospectra were restricted to Schrödinger operators with smooth (at least continuous) potentials. On the other hand, the simplicity of the model enables one to study the spectral and pseudospectral properties of H in a great detail.

It is easy to see that the numerical range of H coincides with the closure of the set

$$\mathcal{S} := [0, +\infty) + i\,(-1, 1)\,.$$

It is also possible to show that the spectrum of H is given by two complex semi-axes

$$\sigma(H) = \sigma_{\mathrm{ess}}(H) = [0, +\infty) + i\,\{-1, +1\}\,.$$

By constructing the resolvent kernel of H, we show a much less evident fact that H possesses a *highly non-trivial pseudospectrum* inside $\mathcal{S}$. Indeed, for each $z \in \mathcal{S}$, there exists a positive constant C depending only on $\Im z$ such that

$$C^{-1}\,\Re z \leq \|(H-z)^{-1}\| \leq C\,\Re z\,. \tag{2.21}$$

Consequently, the resolvent norm tends to infinity as $\Re z \to \infty$ inside $\mathcal{S}$. For a numerical computation of the pseudospectrum of this model, see Figure 21.1 (courtesy of M. Embree).

In [42] we also study the influence of (2.21) on *spectral instabilities* of H. More specifically, we show that the perturbed operator $H + \varepsilon V$ with $V : \mathbb{R} \to \mathbb{C}$ may possess discrete eigenvalues with the distance to the spectrum of H bounded from below by a positive constant (independent of ε) for all small ε. Explicit examples of piece-wise constant and Dirac potentials are presented.

2.3.3 Pseudomodes

An equivalent characterisation of the pseudospectrum (1.11) of a closed operator H is given by

$$\sigma_\varepsilon(H) = \sigma(H) \cup \left\{ z \in \mathbb{C} : \ \exists \psi \in \mathsf{D}(H),\ \|(H-z)\psi\| < \varepsilon\, \|\psi\| \right\},$$

where the number z and the vector ψ are respectively called the *pseudoeigenvalue* (or *approximate eigenvalue*) and *pseudoeigenvector* (or *pseudomode*). Locating the pseudospectrum of H thus consists in finding the spectrum and the set of pseudoeigenvalues (the latter depends on ε).

Given a complex-valued function $V \in L^2_{\mathrm{loc}}(\mathbb{R})$, let us consider the Schrödinger operator

$$H := -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x) \qquad \text{in} \qquad L^2(\mathbb{R}) \tag{2.22}$$

on its maximal domain. There exists by now a quite extensive literature on *semiclassical pseudospectrum* of non-self-adjoint Schrödinger operators, see notably the pioneering work [15] and the subsequent improvements [17, 67]. This approach consists in introducing an artificial small parameter $\hbar^2$ in front of the kinetic part of the potential

$$H_\hbar := -\hbar^2 \frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x) \qquad \text{in} \qquad L^2(\mathbb{R}) \tag{2.23}$$

and in looking for *semiclassical pseudomodes* $\psi_\hbar$ and *pseudoeigenvalues* $z_\hbar$ of $H_\hbar$, which means that the limit $\|(H_\hbar - z_\hbar)\psi_\hbar\|/\|\psi_\hbar\| \to 0$ holds as $\hbar \to 0$. This construction is perturbative, based on the Liouville-Green approximation, also known as the JWKB method. By scaling for some special potentials (like for instance for the imaginary cubic oscillator (1.6) as explained above), it is possible to use these semiclassical pseudomodes for showing that there are pseudomodes corresponding to large energies of the original operator (2.22). Unfortunately, this scaling approach is typically limited to polynomial-type potentials. Moreover, the standard perturbative approach requires that the potential V is at least continuous to construct a semiclassical pseudomode.

The objective of our joint paper [44] (Chapter 22) with P. Siegl is to develop a *systematic non-semiclassical approach* for constructing pseudomodes of (2.22) corresponding to large pseudoeigenvalues. We achieve in covering a wide class of previously inaccessible potentials, including discontinuous ones. Applications of the results to higher-dimensional Schrödinger operators are also discussed in [44].

In fact, we were initially motivated by the simple example (2.20) where the potential is discontinuous and, moreover, the operator does not have a semiclassical counterpart (meaning that the version of (2.23) with $V(x) := i\,\mathrm{sgn}(x)$ is just equivalent to (2.22)). However, much more general potentials are covered by [44]. It is also worth mentioning that in this paper we eventually solve an open problem raised during the 2015 AIM workshop [1, Open Problem 10.1].

The main approach of [44] is again based on the JWKB method, but now we consider the inverse of the spectral parameter $z \in \mathbb{C}$ as a small parameter. The idea is as follows. If V were constant, *i.e.* $V(x) = V_0$ for all $x \in \mathbb{R}$, exact solutions of the differential equation $-g'' + V_0 g = zg$ would be given by

$$e^{\pm i \int_0^x \sqrt{z - V_0}\,\mathrm{d}t}\,. \tag{2.24}$$

For a variable potential V, we still take (2.24) with V_0 replaced by V as a basic Ansatz to get approximate solutions to $H\psi = z\psi$ as $\Re z \to \infty$. Nonetheless, usually more terms are needed for unbounded potentials or when V is sufficiently regular and more information on the decay rates are sought. In general, we therefore take

$$g(x) := \exp\left(-\sum_{k=-1}^{n-1} z^{-k/2}\, \psi_k(x) \right) \tag{2.25}$$

with some natural number $n \geq 0$. Here functions ψ_k are determined by $n+1$ ordinary differential equations obtained after requiring that the terms in the expression $G(z) := -g'' + Vg - zg$ corresponding to the lowest powers of z vanish. Not surprisingly, ψ_{-1} is determined by and eikonal-type equation an reads $\psi_{-1}(x) := iz^{-1/2} \int_0^x \sqrt{z - V(t)}\, \mathrm{d}t$. The goal is to end up with a negative power of z in $G(z)$ representing the decay of the pseudomode as $\Re z \to \infty$. For larger n one gets a better decay rate, but the price to pay is a higher regularity of V.

To obtain admissible pseudomodes, the procedure above is additionally complicated by employing a *z-dependent cut-off* of the basic Ansatz (2.24). There are also some other technical complications, typically related to unbounded potentials. In fact, one of the main contributions of [44] is the determination of a right class of admissible potentials for which the perturbative scheme works. Instead of presenting the general hypotheses to be found in Chapter 22, here we just mention the following illustrative examples covered by [44]: all polynomial potentials of the form $V(x) := x^\beta + ix^\gamma$ with $\gamma \geq 0$ odd and $\gamma > (\beta-2)/2$ and their perturbations (in particular (1.6) and (2.19) are covered); exponential potentials of the form $V(x) := \alpha \cosh(x) + i \sinh(x)$ with $\alpha \geq 0$; smooth version $V(x) := i \arctan(x)$ of the imaginary sign potential (2.20); and many others.

To include discontinuous potentials, we develop a robust method of *z-dependent mollifications*. This new idea enables us to particularly cover the imaginary sign potential (2.20) and even its unbounded step-like versions.

Finally, let us mention that the semiclassical pseudomodes follow as a special case of our more general approach.

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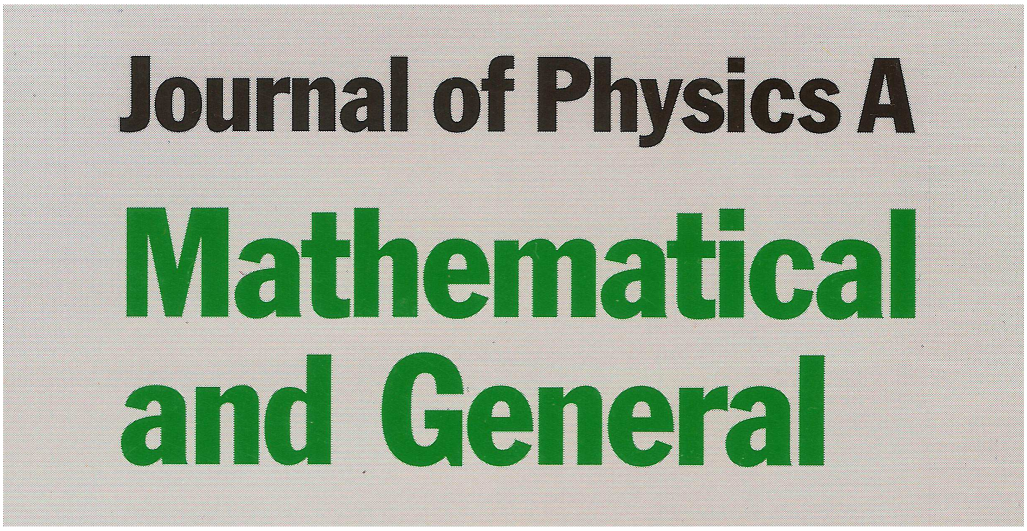
Part I

Toy models

Chapter 3

Closed formula for the metric in the Hilbert space of a $\mathcal{PT}$-symmetric model



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Closed formula for the metric in the Hilbert space of a $\mathcal{PT}$-symmetric model

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Abstract. We introduce a very simple, exactly solvable $\mathcal{PT}$-symmetric non-Hermitian model with real spectrum, and derive a closed formula for the metric operator which relates the problem to a Hermitian one.

3.1 Introduction

In a way motivated by the needs of nuclear physics, Scholtz, Geyer and Hahne [1] established a general mathematical framework for the consistent formulation of quantum mechanics where a set of observables are represented by bounded non-Hermitian operators $A_1, \ldots, A_N$ with real spectra in a Hilbert space $\mathcal{H}$. In essence, they conjectured that in the similar situations one may find a bounded positive Hermitian operator Θ, called *metric*, which fulfils

$$A_k^* \Theta = \Theta A_k \qquad \text{for all} \qquad k \in \{1, \ldots, N\}\,, \tag{3.1}$$

where A_k^* denotes the adjoint operator of A_k in $\mathcal{H}$.

Several years later, the notion of the metric operator Θ re-emerged as a particularly useful mathematical tool in the context of the so-called $\mathcal{PT}$-*symmetric* quantum mechanics [2, 3]. In this framework people usually paid attention to the systems with a single observable, *viz*, with a Hamiltonian $A_1 \equiv H \neq H^*$ which possesses real spectrum and for which the Schrödinger equation is invariant under a simultaneous change of spatial reflection $\mathcal{P}$ and time reversal $\mathcal{T}$.

In the current literature a lot of effort has been devoted to the study of the particular models of H. For their more detailed reviews and discussion the reader is referred to the proceedings of the *International Workshops on Pseudo-Hermitian Hamiltonians in Quantum Physics* [4, 5, 6]. One finds that the construction of a non-trivial operator $\Theta \neq I$, however difficult, is a key to the correct probabilistic interpretation of all the $\mathcal{PT}$-symmetric quantum systems [7, 8, 9, 10]. Indeed, it defines “the physical” inner product $(\cdot,\cdot)_\Theta := (\cdot, \Theta\,\cdot)$ which makes the Hamiltonian H “Hermitian” or, in the language of [1], *quasi-Hermitian.* For this reason, there have been many attempts to calculate the metric operator Θ for the various $\mathcal{PT}$-symmetric models of interest [11, 12, 13, 14, 15, 16, 17, 18, 19]. Because of the complexity of the problem, however, it is not surprising that most of the available formulae for Θ are just approximative, usually expressed as leading terms of perturbation series [17].

The authors of [1] discussed why our knowledge of the new inner product was necessary for the evaluation of the physical predictions. They emphasized that the theory endowed with it is a genuine quantum theory satisfying all the necessary postulates. In a fairly recent continuation of this discussion [20] it has been underlined that in the infinite-dimensional Hilbert spaces $\mathcal{H}$ the requirement of the boundedness of the metric operator Θ plays a key role and that it deserves an extremely careful analysis in the applications where a naïve approach may lead to wrong results. In some sense, our present paper may be read as a direct continuation of the rigorous mathematical discussion in [20].

In particular we are going to illustrate here that our understanding of (3.1) for unbounded operators H as the identity on functions from the operator domain of H (*cf* (3.9) below) requires that Θ maps the operator domain of H into the operator domain of the adjoint H^*. In such a setting we imagined that the best way of finding a support for such an argument can be sought in some exactly solvable $\mathcal{PT}$-symmetric model. We decided to develop a new one – such that its metric can be obtained in a closed formula and in a rigorous manner.

The model we deal with in the present paper is one-dimensional, defined in the Hilbert space

$$\mathcal{H} := L^2\big((0,d)\big)$$

where d is a given positive number. In this Hilbert space we consider the Hamiltonian H_α which acts as the Laplacian, *i.e.*,

$$H_\alpha \psi := -\psi''\,,$$

and satisfies the following Robin boundary conditions:

$$\psi'(0) + i\alpha\,\psi(0) = 0 \qquad \text{and} \qquad \psi'(d) + i\alpha\,\psi(d) = 0\,. \tag{3.2}$$

Here ψ is a function from the Sobolev space $W^{2,2}((0,d))$ and α is a real constant. That is, the operator domain $\mathsf{D}(H_\alpha)$ consists of functions with integrable (generalized) derivatives up to the second order and satisfying (3.2) at the boundary points. Because of the nature of the boundary conditions, H_α is not Hermitian unless $\alpha = 0$, but it is $\mathcal{PT}$-symmetric with the operators $\mathcal{P}$ and $\mathcal{T}$ being defined by $(\mathcal{P}\psi)(x) := \psi(d-x)$ and $\mathcal{T}\psi := \overline{\psi}$, respectively.

It seems that our Hamiltonian H_α represents the simplest $\mathcal{PT}$-symmetric model whatsoever. The fact that the support of the non-Hermitian perturbation is of measure zero invokes the $\mathcal{PT}$-symmetric models [21, 22, 23] involving complex point interactions. But our model is even simpler, since it does not require any matching of solutions known explicitly off the points where the δ-interaction is supported.

Indeed, the non-Hermiticity of H_α enters through the boundary conditions only, while the Hamiltonian models a free quantum particle in the interval $(0,d)$. Consequently, the spectral problem for H_α can be solved explicitly in terms of sines and cosines (*cf* Section 3.3 for more details). Furthermore, an explicit form for the eigenfunctions enables us to obtain a remarkably simple expression for the metric operator:

Theorem 3.1. *Let $\Theta(\alpha)$ be the linear operator defined in $\mathcal{H}$ by*

$$\Theta(\alpha) := I + \phi_0^\alpha\,(\phi_0^\alpha,\cdot) + \Theta_0 + i\alpha\,\Theta_1 + \alpha^2\Theta_2\,, \tag{3.3}$$

where I denotes the identity operator in $\mathcal{H}$, $(\cdot,\cdot)$ is the inner product on $\mathcal{H}$, antilinear in the first factor and linear in the second one,

$$\phi_0^\alpha(x) := \sqrt{\frac{1}{d}}\,\exp{(i\alpha x)} \tag{3.4}$$

and the operators Θ_0, Θ_1 and Θ_2 acts in $\mathcal{H}$ as

$$(\Theta_0\psi)(x) := -\frac{1}{d}\,(J\psi)(d)\,, \tag{3.5}$$

$$(\Theta_1\psi)(x) := 2\,(J\psi)(x) - \frac{x}{d}\,(J\psi)(d) - \frac{1}{d}\,(J^2\psi)(d)\,, \tag{3.6}$$

$$(\Theta_2\psi)(x) := -(J^2\psi)(x) + \frac{x}{d}\,(J^2\psi)(d)\,, \tag{3.7}$$

with

$$(J\psi)(x) := \int_0^x \psi\,. \tag{3.8}$$

Then $\Theta(\alpha)$ is bounded, symmetric, non-negative and satisfies

$$\forall \psi \in \mathsf{D}(H_\alpha), \qquad H_\alpha^*\,\Theta(\alpha)\,\psi = \Theta(\alpha)\,H_\alpha\,\psi\,. \tag{3.9}$$

Furthermore, $\Theta(\alpha)$ is positive if the condition

$$\alpha d/\pi \;\notin\; \mathbb{Z}\backslash\{0\} \tag{3.10}$$

holds true.

Note that the metric $\Theta(\alpha)$ tends to the identity operator I as $\alpha \to 0$, which is expected due to the fact that H_0 is nothing else than the (self-adjoint) Neumann Laplacian in $\mathcal{H}$. The condition (3.10) ensures that all the eigenvalues of H_α are simple. For simplicity, we do not consider the degenerate cases in the present paper.

This paper is organized as follows. In the following Section 3.2 we introduce the Hamiltonian H_α by means of its associated quadratic form; this provides an elegant way of showing that the operator is closed. The spectral problem for H_α is considered in Section 3.3; in particular, we show that the spectrum is real and discrete, and write down the explicit eigenfunctions and eigenvalues. Section 3.4 contains the main idea of the present paper; namely, we observe that the eigenfunctions of H_α are expressed in terms of Dirichlet and Neumann complete orthonormal families in the interval $(0,d)$ and use a special normalization to simplify the eigenfunctions of the adjoint H_α^*. These enable us, in Section 3.5, to evaluate certain infinite series defining the metric operator and prove Theorem 3.1. We conclude the paper by Section 3.6 where we add several remarks and discuss a possible extension of our model.

3.2 The Hamiltonian

Let us first introduce the operator H_α in a proper way. We start with the associated sesquilinear form h_α defined in the Hilbert space $\mathcal{H}$ by the domain $\mathsf{D}(h_\alpha) := W^{1,2}((0,d))$ and by the prescription:

$$h_\alpha(\phi,\psi) := (\phi',\psi') + i\alpha\,\overline{\phi(d)}\,\psi(d) - i\alpha\,\overline{\phi(0)}\,\psi(0)\,. \tag{3.11}$$

Here $(\cdot,\cdot)$ denotes the standard inner product on $\mathcal{H}$; the corresponding norm will be denoted by $\|\cdot\|$.

Note that the boundary terms in (3.11) are well defined because the domain of the quadratic form is embedded in the space of uniformly continuous functions on $(0,d)$ due to the Sobolev embedding theorem [24]. It is also known that the Sobolev space $W^{1,2}((0,d))$ is dense in $\mathcal{H}$; hence h_α is densely defined. Moreover, the real part of h_α, denoted by $\Re h_\alpha$, is a densely defined, symmetric, positive, closed sesquilinear form (since it corresponds to the self-adjoint Neumann Laplacian in $\mathcal{H}$). Of course, h_α itself is not symmetric unless $\alpha = 0$, however, it can be shown that it is sectorial and closed. To see it, we use [25, Thm. VI.1.33] and prove that the imaginary part of h_α, denoted by $\Im h_\alpha$, is a small perturbation of $\Re h_\alpha$ in the following sense:

Lemma 3.1. *$\Im h_\alpha$ is relatively bounded with respect to $\Re h_\alpha$, with*

$$\big|(\Im h_\alpha)[\psi]\big| \le \epsilon^{-1}\,\alpha^2\,\|\psi\|^2 + \epsilon\,(\Re h_\alpha)[\psi]$$

for all $\psi \in W^{1,2}((0,d))$ and any positive constant ϵ.

Proof. Writing $|\psi(d)|^2 - |\psi(0)|^2 = \int_0^d \big(|\psi|^2\big)' = 2\,\Re\big(\psi,\psi'\big)$, and applying the Schwarz and Cauchy inequalities to the last term, we obtain the desired result. □

In view of the above properties and the first representation theorem [25, Thm. VI.2.1], there exists a unique m-sectorial operator H_α in $\mathcal{H}$ such that $h_\alpha(\phi,\psi) = (\phi, H_\alpha\psi)$ for all $\phi \in \mathsf{D}(h_\alpha)$ and $\psi \in \mathsf{D}(H_\alpha) \subset \mathsf{D}(h_\alpha)$. The operator domain $\mathsf{D}(H_\alpha)$ consists of those functions $\psi \in \mathsf{D}(h_\alpha)$ for which there exists $\eta \in \mathcal{H}$ such that $h_\alpha(\phi,\psi) = (\phi,\eta)$ holds for every $\phi \in \mathsf{D}(h_\alpha)$. Furthermore, using the ideas of [25, Ex. VI.2.16], it is possible to verify that indeed

$$\begin{aligned} H_\alpha\psi &= -\psi''\,, \\ \psi \in \mathsf{D}(H_\alpha) &= \big\{\psi \in W^{2,2}((0,d)) \mid \psi \text{ satisfies (3.2)}\big\}\,. \end{aligned} \tag{3.12}$$

The above procedure also implies that the adjoint operator H_α^* is simply obtained by the replacement $\alpha \mapsto -\alpha$.

Summing up the results, we obtain:

Proposition 3.1. *The operator H_α defined by (3.12) is m-sectorial in $\mathcal{H}$ and satisfies*

$$H_\alpha^* = H_{-\alpha}\,.$$

3.3 The spectrum

An important property of an operator being m-sectorial is that it is closed. Then, in particular, the spectrum is well defined by means of the resolvent operator. We claim that our H_α is an operator with compact resolvent. This can be seen by noticing that the Neumann Laplacian H_0 (associated with $\Re h_\alpha$) is an operator with compact resolvent and by using the perturbation result of [25, Thm. VI.3.4] together with Lemma 3.1. Consequently, we know that the spectrum of H_α, denoted by $\sigma(H_\alpha)$, is purely discrete, *i.e.*, it consists entirely of isolated eigenvalues with finite (algebraic) multiplicities.

The eigenvalue problem $H_\alpha\psi = k^2\psi$, with $k \in \mathbb{C}$, can be solved explicitly in terms of sines and cosines. In particular, the boundary conditions lead to the following implicit equation for the eigenvalues:

$$(k^2 - \alpha^2)\,\sin(kd) = 0\,. \tag{3.13}$$

That is,

$$\sigma(H_\alpha) = \big\{\alpha^2\big\} \cup \big\{k_j^2\big\}_{j=1}^{\infty}\,, \qquad \text{where} \qquad k_j := j\pi/d\,. \tag{3.14}$$

Hereafter we shall use the index $j \in \mathbb{N}$ to count the eigenvalues as in (3.14), with the convention that the eigenvalue for $j = 0$ is given by α^2.

While the spectrum of H_α is real, it exhibits important differences with respect to the spectra of self-adjoint one-dimensional differential operators. For instance, the spectrum of H_α may not be simple and even the lowest eigenvalue may be degenerate for particular choices of α. Notice also that H_α coincides with the spectrum of the Neumann Laplacian H_0 up to the lowest (zero) eigenvalue which is shifted to α^2.

In this paper we restrict to the non-degenerate case, *i.e.*, we make the hypothesis (3.10). Then the eigenfunctions of H_α corresponding to (3.14) with the convention mentioned there are given by

$$\psi_j^\alpha(x) := \begin{cases} A_0^\alpha \exp\left(-i\alpha x\right) & \text{if} \quad j=0\,, \\ A_j^\alpha \left(\cos(k_j x) - i\frac{\alpha}{k_j}\sin(k_j x)\right) & \text{if} \quad j \geq 1\,, \end{cases} \tag{3.15}$$

where each A_j is an arbitrary non-zero complex number. In view of Proposition 3.1, the spectrum of the adjoint H_α^* coincides with (3.14) and the corresponding eigenfunctions are given by

$$\phi_j^\alpha(x) := \begin{cases} B_0^\alpha \exp\left(i\alpha x\right) & \text{if} \quad j=0\,, \\ B_j^\alpha \left(\cos(k_j x) + i\frac{\alpha}{k_j}\sin(k_j x)\right) & \text{if} \quad j \geq 1\,, \end{cases} \tag{3.16}$$

where each B_j is again an arbitrary non-zero complex number.

We collect the obtained spectral results into the following proposition:

Proposition 3.2. *The spectrum of H_α is real and consists of discrete eigenvalues specified in (3.14). If the condition (3.10) holds, then all the eigenvalues have multiplicity one and the corresponding eigenfunctions are given by (3.15).*

3.4 Special normalization

It follows directly by combining the eigenvalue problems for H_α and its adjoint that ϕ_j^α and ψ_k^α are orthogonal to each other provided $j \neq k$ and the non-degeneracy condition (3.10) holds. The stronger result

$$\forall j,k \in \mathbb{N}, \quad (\phi_j^\alpha, \psi_k^\alpha) = \delta_{jk} \tag{3.17}$$

will hold provided we normalize the eigenfunctions in a special way. Namely, (3.17) follows by choosing the coefficients A_j^α and B_j^α according to the equations

$$1 = A_0^\alpha\, \overline{B_0^\alpha}\, \frac{1-\exp(-2i\alpha d)}{2i\alpha}\,, \tag{3.18}$$

$$1 = A_j^\alpha\, \overline{B_j^\alpha}\, \frac{(k_j^2-\alpha^2)\, d}{2k_j^2} \qquad \text{for} \quad j \geq 1\,. \tag{3.19}$$

(If $\alpha = 0$, the fraction in the first equation should be understood as the expression obtained after taking the limit $\alpha \to 0$.) These equations can clearly be satisfied as soon as (3.10) holds.

We still have a freedom in specifying A_j^α and B_j^α. For further purposes, however, we choose the coefficients B_j^α in a very simple form by the requirements

$$B_0 := \sqrt{1/d} \qquad \text{and} \qquad B_j := \sqrt{2/d} \qquad \text{for} \quad j \geq 1\,, \tag{3.20}$$

while we leave more complicated formula, determined by the equations (3.18) and (3.19), for the coefficients A_j^α. Then ϕ_0^α coincides with (3.4) and we have the decomposition

$$\phi_j^\alpha(x) = \chi_j^N(x) + i\frac{\alpha}{k_j}\,\chi_j^D(x) \qquad \text{for} \quad j \geq 1\,, \tag{3.21}$$

where $\{\chi_j^N\}_{j=0}^\infty$, respectively $\{\chi_j^D\}_{j=1}^\infty$, denotes the set of normalized eigenfunctions of the Neumann, respectively Dirichlet, Laplacian in $\mathcal{H}$:

$$\chi_j^N(x) := \begin{cases} \sqrt{1/d} & \text{if} \quad j=0\,, \\ \sqrt{2/d}\,\cos(k_j x) & \text{if} \quad j \geq 1\,, \end{cases} \qquad \chi_j^D(x) := \sqrt{2/d}\,\sin(k_j x)\,.$$

In addition to (3.21), we also have the uniform convergence $\phi_0^\alpha \to \chi_0^N$ as $\alpha \to 0$. We point out the result we shall need later:

Proposition 3.3. *If the condition (3.10) holds true, then the eigenfunctions ψ_j^α of H_α and the eigenfunctions ϕ_j^α of H_α^* can be chosen in such a way that they satisfy the biorthonormality relations (3.17) and the latter satisfy (3.21).*

The decomposition (3.21) plays a crucial role in the subsequent section, mainly due to the fact that $\{\chi_j^N\}_{j=0}^{\infty}$ and $\{\chi_j^D\}_{j=1}^{\infty}$ are well known to form *complete orthonormal families*. In particular, we have the expansions

$$\psi = \sum_{j=0}^{\infty} \chi_j^N \, (\chi_j^N, \psi) = \sum_{j=1}^{\infty} \chi_j^D \, (\chi_j^D, \psi) \tag{3.22}$$

and the Parseval equalities

$$\|\psi\|^2 = \sum_{j=0}^{\infty} |(\chi_j^N, \psi)|^2 = \sum_{j=1}^{\infty} |(\chi_j^D, \psi)|^2 \tag{3.23}$$

for every $\psi \in \mathcal{H}$.

3.5 The metric

With an abuse of notation, we initially define

$$\Theta(\alpha) := \sum_{j=0}^{\infty} \phi_j^{\alpha} \, (\phi_j^{\alpha}, \cdot) \tag{3.24}$$

and show that this operator can be cast into the form (3.3) with (3.4)–(3.7). In fact, using (3.21) and (3.22), it is readily seen that (3.3) holds with

$$\Theta_0 := -\chi_0^N \, (\chi_0^N, \cdot) \tag{3.25}$$

and

$$\Theta_1 := \sum_{j=1}^{\infty} \frac{\chi_j^D \, (\chi_j^N, \cdot) - \chi_j^N \, (\chi_j^D, \cdot)}{k_j} \,, \qquad \Theta_2 := \sum_{j=1}^{\infty} \frac{\chi_j^D \, (\chi_j^D, \cdot)}{k_j^2} \,. \tag{3.26}$$

Recalling the definition (3.8) of the bounded integral operator J in $\mathcal{H}$, it is evident that the rank-one operator (3.25) can be expressed in terms of J as in (3.5). It remains to verify that (3.26) can be expressed as in (3.6) and (3.7).

First of all, we notice that the operator (3.24) is well defined in the sense that Θ_1 and Θ_2 as defined in (3.26) are bounded linear operators in $\mathcal{H}$. This can be seen by using (3.23) and the Schwarz inequality. Actually, the series in (3.26) are uniformly convergent, and Θ_2 can be written as an integral Hilbert-Schmidt operator, but we will not use these facts. Our way to sum up the infinite series is based on the following lemma:

Lemma 3.2.

$$\sum_{j=1}^{\infty} \frac{\chi_j^D(x)\, \chi_j^N(d)}{k_j} = -\frac{x}{d} \qquad \textit{uniformly for all} \quad x \in [0,d] \,.$$

Proof. The series is uniformly convergent due to Abel's uniform convergence test. Let l denote the identity function on $(0,d)$, *i.e.* $l(x) := x$. Using the expansion (3.22) and integrating by parts, we get

$$l = \sum_{j=1}^{\infty} \chi_j^D \, (\chi_j^D, l) = \sum_{j=1}^{\infty} \chi_j^D \, \big((-\chi_j^N/k_j)', l\big) = -\sum_{j=1}^{\infty} \chi_j^D \, \chi_j^N(d) \, d/k_j \,,$$

where the last equality follows from the fact that all χ_j^N with $j \geq 1$ are orthogonal to the constant function χ_0^N. This concludes the proof. □

Since $J\psi$ is an indefinite integral of ψ and $(J\psi)(0) = 0$, an integration by parts yields for every $\psi \in \mathcal{H}$:

$$(\chi_j^N, \psi) = k_j \, (\chi_j^D, J\psi) + \chi_j^N(d) \, (J\psi)(d) \,,$$
$$(\chi_j^D, \psi) = -k_j \, (\chi_j^N, J\psi) = -k_j^2 \, (\chi_j^D, J^2\psi) - k_j \, \chi_j^N(d) \, (J^2\psi)(d) \,.$$

Incorporating these identities into (3.26) and using (3.22) together with Lemma 3.2, we obtain the formulae (3.6) and (3.7) for (3.26).

Now we are in a position to prove Theorem 3.1.

Proof of Theorem 3.1. The boundedness of (3.3) is clear; in particular, crude estimates yield

$$\|\Theta(\alpha)\psi\| \leq (3 + 4\alpha d + 2\alpha^2 d^2)\,\|\psi\|$$

for every $\psi \in \mathcal{H}$.

Integrating by parts, it is also easy to check that the identity

$$\big(\psi, \Theta(\alpha)\psi\big) = |(\phi_0^\alpha, \psi)|^2 + \|\psi + i\alpha J\psi\|^2 - |(\chi_0^N, \psi + i\alpha J\psi)|^2 \tag{3.27}$$

holds for every $\psi \in \mathcal{H}$, where the right hand side is real-valued and non-negative due to (3.23). This proves that $\Theta(\alpha)$ is symmetric and non-negative.

Let us show that $\Theta(\alpha)$ is positive provided (3.10) holds. If the right hand side of (3.27) were equal to zero with a non-zero $\psi \in \mathcal{H}$, then the first Parseval equality in (3.23) would imply that the function $\psi + i\alpha J\psi$ must be constant, being orthogonal to all functions orthogonal to 1. Consequently, ψ is proportional to ψ_0^α and an explicit calculation yields

$$|(\phi_0^\alpha, \psi)| = \left|\frac{\sin(\alpha d)}{\alpha d}\right| \|\psi\|\,,$$

which is clearly positive for all α satisfying (3.10).

Finally, let us comment on the identity (3.9). Let $\psi \in \mathsf{D}(H_\alpha)$. We first note that it straightforward to check that $\Theta(\alpha)\psi$ belongs to $\mathsf{D}(H_\alpha^*)$, so that the left hand side of (3.9) makes sense. We also have

$$-(\Theta(\alpha)\,\psi)'' = -\psi'' - 2i\alpha\psi' + \alpha^2\psi + \alpha^2\phi_0^\alpha(\phi_0^\alpha, \psi) = -\Theta(\alpha)\psi''\,.$$

Here the first equality follows at once, while the second one is not trivial, but it can be verified by using a number of integrations by parts.

This concludes the proof of Theorem 3.1. □

3.6 Concluding remarks

3.6.1 Alternative proofs of the reality of the spectrum

Recall that $\mathcal{PT}$-symmetry itself is not sufficient to guarantee the reality of the spectrum of a non-Hermitian operator (see, *e.g.*, [26, 27]). Moreover, the existing proofs of the reality [28, 29, 30, 31] are based on rather advanced techniques. Therefore we find it interesting that the reality of the eigenvalues of our Hamiltonian H_α can be deduced directly from the structure of the operator, without solving the eigenvalue problem explicitly.

To see it, we rewrite the eigenvalue problem $H_\alpha\psi = k^2\psi$ using the unitary transform $\psi \mapsto \phi_0^\alpha\psi := \phi$ into the boundary value problem

$$\begin{cases} -\phi'' + 2i\alpha\phi' + \alpha^2\phi = k^2\phi & \text{in} \quad (0,d)\,, \\ \qquad\qquad\qquad\quad \phi' = 0 & \text{at} \quad 0, d\,. \end{cases} \tag{3.28}$$

Now we multiply the first equation in (3.28) by $\overline{\phi''}$ and integrate over $(0,d)$. We also multiply the complex conjugation of the first equation in (3.28) by ϕ'' and integrate over $(0,d)$. Then we subtract the results and use various integrations by parts together with the Neumann boundary conditions to get the identity

$$\Im(k^2)\,\|\phi'\|^2 = 0\,.$$

Consequently, either the eigenvalue k^2 is real or the corresponding eigenfunction ϕ is constant. It remains to realize that also the latter implies the former in view of (3.28).

Finally, let us mention that H_α can be reconsidered as a self-adjoint operator in a Krein space [29]. Then the reality of the spectrum of H_α for $|\alpha| < \pi/d$ follows from [29, Corol. 3.3]. An alternative proof of the reality of the spectrum of H_α for small α also follows from the perturbation result of [30].

3.6.2 Biorthonormal basis

It is easily seen that the operator $\Theta(\alpha)$ defined by (3.24) formally satisfies (3.9), with the inverse given by $\Theta(\alpha)^{-1} = \sum_{j=0}^\infty \psi_j^\alpha\,(\psi_j^\alpha, \cdot)$, provided $\{\psi_j^\alpha\}_{j=0}^\infty$ and $\{\phi_j^\alpha\}_{j=0}^\infty$ fulfil in addition to (3.17) the following biorthonormal-basis-type relation:

$$\forall \psi \in \mathcal{H}, \qquad \psi = \sum_{j=0}^\infty \psi_j^\alpha\,(\phi_j^\alpha, \psi)\,. \tag{3.29}$$

By "formally" we mean that one has to justify an interchange of summation and differentiation. We did not pursue this direction in the present paper. Instead, we summed up the infinite series (3.24) using the special normalization (3.20) leading to (3.21), and checked that the resulting operator indeed satisfies (3.1) in the sense of (3.9).

Nevertheless, let us show that the expansion (3.29) holds:

Proposition 3.4. *If the condition (3.10) holds true, then the eigenfunctions ψ_j^α of H_α and the eigenfunctions ϕ_j^α of H_α^* can be chosen in such a way that (3.29) is satisfied.*

Proof. Assume the special normalization of Section 3.4. Let us first verify that $\{\psi_j\}_{j=0}^\alpha$ is a basis of $\mathcal{H}$, *i.e.*,

$$\forall \psi \in \mathcal{H}, \qquad \psi = \sum_{j=0}^{\infty} c_j^\psi \, \psi_j^\alpha \,, \tag{3.30}$$

where $\{c_j^\psi\}_{j=0}^\infty$ is a unique sequence of complex numbers. Note that the equality in (3.30) should be understood as a limit in the norm topology of $\mathcal{H}$; in particular, (3.30) implies the weak convergence

$$\forall \phi, \psi \in \mathcal{H}, \qquad (\phi, \psi) = \lim_{m\to\infty} \left(\phi, \sum_{n=1}^{m} c_j^\psi \, \psi_j^\alpha\right). \tag{3.31}$$

Substituting $\psi = 0$ and $\phi = \phi_k^\alpha$, $k \in \mathbb{N}$, into (3.31), the biorthonormality relations (3.17) yield that (3.30) with $\psi = 0$ implies that all $c_j^0 = 0$. At the same time,

$$\|\psi_j^\alpha - \chi_j^N\|^2 = \alpha^2 \, \frac{k_j^2 + \alpha^2}{(k_j^2 - \alpha^2)^2} \qquad \text{for} \quad j \geq 1$$

and since the right hand side behaves as $\mathcal{O}(j^{-2})$ as $j \to \infty$, we have

$$\sum_{j=0}^{\infty} \|\psi_j^\alpha - \chi_j^N\|^2 < \infty \,.$$

Consequently, $\{\psi_j\}_{j=0}^\alpha$ is a basis of $\mathcal{H}$ due to [25, Thm. V.2.20]. Finally, substituting $\phi = \phi_k^\alpha$, $k \in \mathbb{N}$, into (3.31), the biorthonormality relations (3.17) yield that $c_j^\psi = (\phi_j^\alpha, \psi)$ for all $j \in \mathbb{N}$. □

The same argument also implies the following expansion:

$$\forall \psi \in \mathcal{H}, \qquad \psi = \sum_{j=0}^{\infty} \phi_j^\alpha \, (\psi_j^\alpha, \psi) \,.$$

3.6.3 A more general model

For simplicity, we required that α was real in the present paper. A more general model is given by the following more general $\mathcal{PT}$-symmetric boundary conditions:

$$\psi'(0) + (\beta + i\alpha)\,\psi(0) = 0 \qquad \text{and} \qquad -\psi'(d) + (\beta - i\alpha)\,\psi(d) = 0 \,, \tag{3.32}$$

where α and β are real constants. A straightforward modification of the approach of Section 3.2 (*cf* also the first paragraph of Section 3.3) yields:

Proposition 3.5. *The operator $H_{\alpha,\beta}$ defined in $\mathcal{H}$ by*

$$\begin{aligned} H_{\alpha,\beta}\,\psi &= -\psi'' \,, \\ \psi \in \mathsf{D}(H_{\alpha,\beta}) &= \left\{\psi \in W^{2,2}((0,d)) \mid \psi \text{ satisfies (3.32)}\right\}, \end{aligned}$$

is an m-sectorial operator with compact resolvent and satisfies $H_{\alpha,\beta}^* = H_{-\alpha,\beta}$.

The eigenvalue problem $H_{\alpha,\beta}\,\psi = k^2\psi$, with $k \in \mathbb{C}$, can again be solved in terms of sines and cosines, and one gets the following implicit equation for the eigenvalues:

$$\left[k^2 - (\alpha^2 + \beta^2)\right] \sin(kd) - 2\,\beta\,k\,\cos(kd) = 0 \,.$$

The main difference with respect to the case $\beta = 0$ studied in the present paper is that $H_{\alpha,\beta}$ can possess non-real complex conjugate eigenvalues for $\beta \neq 0$.

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Chapter 4

Calculation of the metric in the Hilbert space of a $\mathcal{PT}$-symmetric model via the spectral theorem

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Calculation of the metric in the Hilbert space of a $\mathcal{PT}$-symmetric model via the spectral theorem

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Abstract. In a previous paper [1] we introduced a very simple $\mathcal{PT}$-symmetric non-Hermitian Hamiltonian with real spectrum and derived a closed formula for the metric operator relating the problem to a Hermitian one. In this note we propose an alternative formula for the metric operator, which we believe is more elegant and whose construction – based on a backward use of the spectral theorem for self-adjoint operators – provides new insights into the nature of the model.

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Keywords: $\mathcal{PT}$-symmetry, metric operator, non-self-adjointness, spectral theorem, Robin boundary conditions

4.1 Introduction

Although quantum mechanic is conceptually a self-adjoint theory, there are numbers of problems that require the analysis of non-self-adjoint operators. The study of resonances of self-adjoint Schrödinger operators via the technique of complex scaling [2] or the derivation of the famous Landau-Zener formula for the adiabatic transition probability between eigenstates of a time-dependent two-level system [3] are just two examples. However, in contrast to the well understood theory of self-adjoint operators, the non-self-adjoint theory can be quite different (*cf* a nice review [4]) and is certainly less developed. The former is much easier to analyse because of the existence of the spectral theorem.

Recent years brought new motivations and focused attention to aspects of problems which attracted little attention earlier. A strong impetus comes from the so-called $\mathcal{PT}$-symmetric quantum mechanics, where the Hamiltonian H of a system is not Hermitian but the Schrödinger equation is invariant under a simultaneous change of spatial reflection $\mathcal{P}$ and time reversal $\mathcal{T}$ (*cf* [5] for the pioneering work and [6] for a recent review with many references). Here the interest consists in the fact that many of the $\mathcal{PT}$-symmetric Hamiltonians possess real spectra and that the problem can be reinterpreted as a Hermitian one in a different Hilbert space. Indeed, and more generally, the identification is provided by the quasi-Hermiticity relation [7, 8, 9, 10]:

$$H^*\Theta = \Theta H \tag{4.1}$$

valid on the domain of H. Here Θ is a bounded positive Hermitian operator, called metric.

There have been many attempts to calculate the metric operator Θ for the various $\mathcal{PT}$-symmetric models of interest (*cf* [1] for related references to which we add the Swanson model [11, 12, 13] and recent works [14, 15]). Most recent developments have come up with new efficient methods how to calculate the metric [16, 17, 18, 19, 20], involving exact (non-perturbative) solutions in a compact form. Because of the complexity of the problem, however, it is not surprising that the majority of the available formulae for Θ are still approximative, usually expressed as leading terms of perturbation series.

Another problematic aspect of the available results is that the calculations are usually formal, partly because the boundedness of Θ is not always verified. However, the boundedness of the metric is a necessary condition, as addressed already in the original paper [7] and further emphasized in [21].

For these reasons we decided in [1] to introduce a new one-parametric non-Hermitian $\mathcal{PT}$-symmetric Hamiltonian H_α with real spectrum and derived a formula for its metric Θ_α in a closed form and in a rigorous manner. The latter were allowed due to the manifest simplicity of our model: Recalling the $\mathcal{PT}$-symmetric operators with general complex point interactions introduced by Albeverio, Fei and Kurasov in [22], our model can be roughly viewed as the Hamiltonian of a potential-free particle constrained to a bounded interval with two point-type interactions 'sitting' at the interval endpoints. In other words, we introduce a non-trivial coupling due to boundary conditions rather than to a local potential term. The calculation of the metric in [1] then relied on the fact that the eigenfunctions of H_α can be expressed explicitly in terms of trigonometric functions. Using the completeness of the latter, the metric operator was constructed by summing up certain trigonometric series.

The ultimate objective of this note is to point out that the series determining Θ_α can be summed up alternatively – and probably more elegantly – by using the spectral theorem. Moreover, we believe that the resulting formula for the metric has a more transparent structure than that presented in [1]. Indeed, the individual terms of the present formula are well-known integral operators with explicit and extremely simple kernels (*cf* Remark 4.2 below). We also hope that the simplicity of the formula will stimulate further study of the quasi-Hermiticity of our model, namely a (perturbative) computation of the square root of the metric operator and the corresponding Hermitian counterpart of H_α.

For the convenience of the reader we state here a simple version of the spectral theorem we shall use later:

Theorem 4.1 (Spectral Theorem)**.** *Let H be a self-adjoint operator with compact resolvent in a Hilbert space with inner product $(\cdot,\cdot)$, antilinear in the first factor and linear in the second one. Then*

$$f(H) = \sum_{j=0}^{\infty} f(E_j)\, \psi_j(\psi_j,\cdot) \tag{4.2}$$

for any complex-valued, continuous function f. Here $\{E_j\}_{j=0}^{\infty}$ and $\{\psi_j\}_{j=0}^{\infty}$ denote respectively the set of eigenvalues and corresponding eigenfunctions of H.

We refer to [23, Sec. VI.5] for a proof and a more general version of the spectral theorem when the compactness assumption is relaxed. Similar spectral decompositions hold also for normal operators, but they are in general false in the non-self-adjoint theory. Therefore it is remarkable that a modified version of (4.2) with $f(E) = E^n$, $n \in \mathbb{N}$, still holds for our non-Hermitian operator H_α (*cf* [1, Prop. 4] for the case $n = 0$, the other cases being a consequence).

The spectral theorem is usually used to construct a function of a self-adjoint operator in terms of the sum of spectral projections. In this note we use it backwards: we identify eigenprojections of a self-adjoint operator and replace an infinite series by a function of the operator. Unfortunately, the present method does not seem to be applicable in general. The reason why it works in the present model is that the eigenfunctions of H_α can be expressed in terms of eigenfunctions of self-adjoint operators.

In the forthcoming Section 4.2 we recall the model introduced in [1] (we refer to that reference for more details and other results). This is followed by Section 4.3 where the alternative formula for the metric is established.

4.2 The model

The underlying Hilbert space of the model introduced in [1] is the space of square-integrable functions $\mathcal{H} := L^2((0,d))$, where d is a positive number. While it is irrelevant that we consider an open interval in the definition of the Hilbert space, this choice turns out to be convenient when defining differential operators in $\mathcal{H}$ via the quadratic-form approach, since the corresponding Sobolev (energy) spaces are standardly defined over open sets only [24].

The simplicity of the Hamiltonian H_α defined in $\mathcal{H}$ consists in that it acts as the potential-free Hamiltonian

$$H_\alpha \psi := -\psi'' \qquad \text{in} \qquad (0,d)\,,$$

while the non-Hermiticity enters uniquely through complex Robin boundary conditions:

$$\psi'(0) + i\alpha\psi(0) = 0 \qquad \text{and} \qquad \psi'(d) + i\alpha\psi(d) = 0\,, \tag{4.3}$$

where α is a real constant. Using the quadratic-form approach, it was shown in [1] that H_α, with the domain $D(H_\alpha)$ consisting of all functions ψ in the Sobolev space $W^{2,2}((0,d))$ such that (4.3) holds, is an m-sectorial operator in $\mathcal{H}$. Note that the boundary terms in (4.3) are well defined because every element of $W^{2,2}((0,d))$ can be identified with a smooth function over $[0,d]$ in the sense of Sobolev embedding theorem [24]. The $\mathcal{PT}$-symmetry of our model is reflected by the relation

$$H_\alpha^* = H_{-\alpha}\,,$$

where H_α^* denotes the adjoint of H_α.

Remark 4.1. A more general class of one-dimensional Schrödinger operators with non-Hermitian boundary conditions of the type (4.3) was studied previously by Kaiser, Neidhardt and Rehberg in [25]. In their paper – motivated by the needs of semiconductor physics, or more generally by regarding a quantum system as an open one – the parameter α is allowed to be complex but its imaginary part has opposite signs on the boundary points such that the system is dissipative. In our case (4.3), we actually deal with radiation/absorption boundary conditions in the language of theory of electromagnetic field.

It was also shown in [1] that the spectrum of H_α is purely discrete and given by

$$\sigma(H_\alpha) = \{\alpha^2\} \cup \{k_j^2\}_{j=1}^{\infty}, \qquad \text{where} \qquad k_j := j\pi/d\,. \tag{4.4}$$

Moreover, all the eigenvalues are simple provided

$$\alpha d/\pi \;\notin\; \mathbb{Z}\backslash\{0\}\,. \tag{4.5}$$

Assuming this non-degeneracy condition, the eigenfunctions of the adjoint H_α^* corresponding to the eigenvalues counted as in (4.4) can be chosen as

$$\phi_j^\alpha(x) := \begin{cases} \chi_0^N + \rho_\alpha(x) & \text{if} \quad j=0\,, \\ \chi_j^N(x) + i\dfrac{\alpha}{k_j}\,\chi_j^D(x) & \text{if} \quad j \geq 1\,. \end{cases} \tag{4.6}$$

Here

$$\rho_\alpha(x) := \frac{\exp(i\alpha x) - 1}{\sqrt{d}}$$

and $\{\chi_j^N\}_{j=0}^\infty$, respectively $\{\chi_j^D\}_{j=1}^\infty$, denotes the complete orthonormal family of the eigenfunctions of the Neumann Laplacian $-\Delta_N$, respectively Dirichlet Laplacian $-\Delta_D$, in $\mathcal{H}$:

$$\chi_j^N(x) := \begin{cases} \sqrt{1/d} & \text{if} \quad j=0\,, \\ \sqrt{2/d}\,\cos(k_j x) & \text{if} \quad j \geq 1\,, \end{cases} \qquad \chi_j^D(x) := \sqrt{2/d}\,\sin(k_j x)\,.$$

Here the index for Dirichlet eigenfunctions runs over $j \geq 1$. Note that $-\Delta_N = H_0$ and that the spectrum of $-\Delta_D$ is equal to $\{k_j^2\}_{j=1}^\infty$.

4.3 Calculation of the metric

Still under the hypothesis (4.5), it was demonstrated in [1] that the operator

$$\Theta_\alpha := \sum_{j=0}^{\infty} \phi_j^\alpha(\phi_j^\alpha,\cdot) \equiv \operatorname*{s\!-\!lim}_{m\to\infty} \sum_{j=0}^{m} \phi_j^\alpha(\phi_j^\alpha,\cdot) \tag{4.7}$$

is bounded, symmetric, positive and satisfying (4.1) with H_α. Here $(\cdot,\cdot)$ denotes the inner product in $\mathcal{H}$, antilinear in the first factor and linear in the second one. Furthermore, a closed integral-type formula for the operator was derived by using known results about the sum of trigonometric functions.

Now we propose an alternative way how to sum up the infinite series in (4.7). First we write Θ_α as

$$\Theta_\alpha = P_0^\alpha + \Theta^{(0)} + \alpha\,\Theta^{(1)} + \alpha^2\,\Theta^{(2)}$$

with

$$\begin{aligned} P_0^\alpha &:= \phi_0^\alpha(\phi_0^\alpha,\cdot) = P_0^N + \chi_0^N(\rho_\alpha,\cdot) + \rho_\alpha(\chi_0^N,\cdot) + \rho_\alpha(\rho_\alpha,\cdot)\,, \\ \Theta^{(0)} &:= \sum_{j=1}^{\infty} \chi_j^N(\chi_j^N,\cdot) = I - P_0^N\,, \\ \Theta^{(1)} &:= \sum_{j=1}^{\infty} \Big(-ik_j^{-1}\,\chi_j^N(\chi_j^D,\cdot) + ik_j^{-1}\,\chi_j^D(\chi_j^N,\cdot)\Big)\,, \\ \Theta^{(2)} &:= \sum_{j=1}^{\infty} k_j^{-2}\,\chi_j^D(\chi_j^D,\cdot) = (-\Delta_D)^{-1}\,, \end{aligned}$$

where $P_0^N := \chi_0^N(\chi_0^N,\cdot) = P_0^0$ and I denotes the identity operator in $\mathcal{H}$. The equalities in the second and fourth lines follow directly by Theorem 4.1 applied to $-\Delta_N$ and $-\Delta_D$, respectively. In order to use the spectral theorem in $\Theta^{(1)}$ as well, we introduce a “momentum” operator p in $\mathcal{H}$ by

$$p\psi := -i\psi'\,, \qquad D(p) := W_0^{1,2}((0,d))\,. \tag{4.8}$$

The adjoint operator p^* acts in the same way but has a larger domain, $D(p^*) = W^{1,2}((0,d))$. Since χ_j^D and χ_j^N belong to $D(p)$ and $D(p^*)$, respectively, we have $p\chi_j^D = -ik_j\chi_j^N$ and $p^*\chi_j^N = ik_j\chi_j^D$. Consequently, Theorem 4.1 yields

$$\begin{aligned}\Theta^{(1)} &= p\sum_{j=1}^{\infty} k_j^{-2}\,\chi_n^D(\chi_n^D,\cdot) + p^*\sum_{j=1}^{\infty} k_j^{-2}\,\chi_n^N(\chi_n^N,\cdot)\\ &= p\,(-\Delta_D)^{-1} + p^*(-\Delta_N^{\perp})^{-1}\,,\end{aligned}$$

where $-\Delta_N^{\perp} := (I-P^N)(-\Delta_N)(I-P^N)$. Notice that the "interchange of summation and differentiation" in the first equality is justified just by the definition of the sum in (4.7) and the distributional derivative in (4.8).

Summing up, we get

Theorem 4.2. *The linear operator Θ_α in $\mathcal{H}$ defined by*

$$\Theta_\alpha = I + P_0^\alpha - P_0^N + \alpha p\,(-\Delta_D)^{-1} + \alpha p^*(-\Delta_N^{\perp})^{-1} + \alpha^2(-\Delta_D)^{-1} \tag{4.9}$$

is bounded, symmetric, non-negative and satisfies (4.1) *with H_α. Furthermore, Θ_α is positive if the condition* (4.5) *holds true.*

Note that the metric Θ_α tends to I as $\alpha \to 0$, which is expected due to the fact that H_0 coincides with the self-adjoint operator $-\Delta_N$.

Remark 4.2. Formula (4.9) can be written exclusively in terms of the operators p and p^* by employing the identities $-\Delta_D = p^*p$ and $-\Delta_N = pp^*$. Note also that the resolvent $(-\Delta_D)^{-1}$ and the reduced resolvent $(-\Delta_N^{\perp})^{-1}$ are integral operators with explicit and extremely simple kernels (*cf* [23, Ex. III.6.21]).

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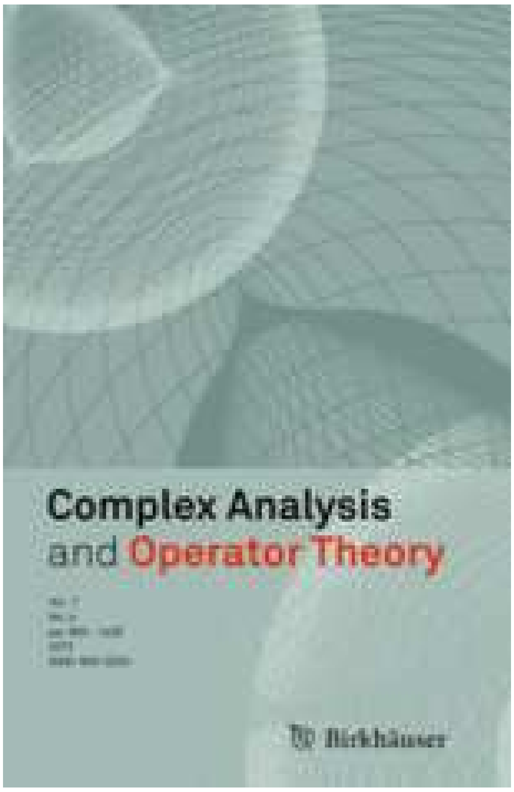
Chapter 5

On the similarity of Sturm-Liouville operators with non-Hermitian boundary conditions to self-adjoint and normal operators



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On the similarity of Sturm-Liouville operators with non-Hermitian boundary conditions to self-adjoint and normal operators

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Abstract. We consider one-dimensional Schrödinger-type operators in a bounded interval with non-self-adjoint Robin-type boundary conditions. It is well known that such operators are generically conjugate to normal operators via a similarity transformation. Motivated by recent interests in quasi-Hermitian Hamiltonians in quantum mechanics, we study properties of the transformations and similar operators in details. In the case of parity and time reversal boundary conditions, we establish closed integral-type formulae for the similarity transformations, derive a non-local self-adjoint operator similar to the Schrödinger operator and also find the associated "charge conjugation" operator, which plays the role of fundamental symmetry in a Krein-space reformulation of the problem.

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5.1 Introduction

Let us consider the m-sectorial realization H of the second derivative operator

$$\psi \mapsto -\psi'' \tag{5.1}$$

in the Hilbert space $\mathcal{H} := L^2(-a,a)$, with $a>0$, subjected to separated, Robin-type boundary conditions

$$\psi'(\pm a) + c_\pm\,\psi(\pm a) = 0 \tag{5.2}$$

where $c_\pm$ are arbitrary complex numbers. The operator H is self-adjoint if, and only if, the constants $c_\pm$ are real. The present paper is concerned with the existence and properties of similarity transformations of H to a normal or self-adjoint operator in the non-trivial case of non-real $c_\pm$.

The similarity to the normal (respectively, self-adjoint) operator is understood as the existence of a bounded operator Ω with bounded inverse such that

$$h := \Omega H \Omega^{-1} \tag{5.3}$$

is normal (respectively, self-adjoint). We remark that this concept is equivalent to the existence of a topologically equivalent inner product in $\mathcal{H}$ with respect to which H is normal (respectively, self-adjoint). We investigate the general properties of the similarity transformations, modified inner products, and transformed operators and we present explicit closed formulae for these objects in special cases of boundary conditions.

Similarity to a normal or self-adjoint operator has been studied both for abstract and particular operators by many authors. For the former, let us mention [38, 45, 35, 4] where resolvent criteria for the similarity were obtained. For the analysis of specific classes of differential operators see *e.g.* [13, Chap.XX.1] for Sturm-Liouville operator defined on the half-line, and [9, 15, 23, 27, 25, 24] and [2] for respectively indefinite and $\mathcal{PT}$-symmetric Sturm-Liouville operators on the whole real line.

The operators of the type (5.1)–(5.2) have been studied from many aspects and there exist a large number of known results; we particularly mention the classical monograph of Dunford and Schwartz [13, Chapter XIX.3]. Recent years brought new motivations and focused attention to some aspects of the problem which attracted little attention earlier.

As an example, let us mention that one-dimensional Schrödinger operators with non-Hermitian boundary conditions of the type (5.2) were used as a model in semiconductor physics by Kaiser, Neidhardt and Rehberg

[22]. In their paper the imaginary parts of the constants $c_\pm$ are required to have opposite signs such that the system is dissipative. The authors find the characteristic function of the operators, construct its minimal self-adjoint dilation and develop the generalized eigenfunction expansion for the dilation. See also [20, 21] for further generalizations. Here the main idea of using non-self-adjointness comes from embedding a quantum-mechanically described structure into a macroscopic flow and regarding the system as an open one.

However, the principal motivation of the present work is the possibility of giving a direct quantum-mechanical interpretation of non-Hermitian operators which are similar to self-adjoint ones [40]. The most recent strong impetus to this point of view comes from the so-called $\mathcal{PT}$-symmetric quantum mechanics. Here the reality of the spectrum of a class of non-Hermitian operators – caused by certain symmetries rather than self-adjointness – suggests their potential relevance as quantum-mechanical Hamiltonians; see the review articles [5, 37]. It has been confirmed during the last years that it is indeed the case provided that the similarity transformation to a self-adjoint operator can be ensured. However, it is a difficult task.

Motivated by the lack of rigorous results, the authors of [30] introduced a simple non-Hermitian $\mathcal{PT}$-symmetric operator of the type (5.1)–(5.2) and wrote down a closed formula for the (square of the) similarity transformation (see also [29, 31]). Let us also mention that the importance of (not only) $\mathcal{PT}$-symmetric version of (5.1)–(5.2) in quantum mechanical scattering has been recently established in [19].

The present paper can be regarded as a step further. In addition to considering more general situations of larger classes of boundary conditions and similarity to normal operators, we provide an alternative and more elegant (integral-kernel) formulae for the similarity transformations in the $\mathcal{PT}$-symmetric situation. Moreover, we also give a remarkably simple formula for the self-adjoint operator (5.3) in this case. Finally, we succeed in finding the so-called $\mathcal{C}$-operator in a closed form, which plays the role of fundamental symmetry in a Krein-space reformulation of the problem.

The distinguished role of $\mathcal{PT}$-symmetry in the present paper can be understood as follows. It makes sense to look for a *self-adjoint* operator similar to that generated by (5.1)–(5.2) only if the spectrum of the latter is *real*. However, the reality of the spectrum is a highly non-trivial property unless (5.1)–(5.2) is already self-adjoint. In general, it is known that $\mathcal{PT}$-symmetry is neither sufficient nor necessary to guarantee that the spectrum of a non-Hermitian operator is real. However, in the present model, it is clear from the eigenvalue asymptotics (5.30) that the equality of the *imaginary* parts of $c_\pm$ is *necessary* to ensure that the spectrum of (5.1)–(5.2) is real and this necessary condition is in fact guaranteed by the $\mathcal{PT}$-symmetry (*cf* Proposition 5.2).

The paper is organised as follows. In Section 5.2 we give a precise definition of the operator H, summarize its known properties and recall the general concepts of quasi-Hermitian, $\mathcal{PT}$-symmetric, and $\mathcal{C}$-symmetric operators. The structure and properties of the similarity transformations and the corresponding similar operators are investigated in Section 5.3. In Section 5.4 we show how these can be applied to particular ($\mathcal{PT}$-symmetric) classes of boundary conditions and we present some explicit constructions of the studied objects. In Section 5.5 we discuss how the results can be extended to bounded and even second-order perturbations of H. Our final Section 5.6 presents a series of concluding remarks.

5.2 Preliminaries

We start with recalling general properties of H and concepts of similarity transformations in Hilbert spaces.

5.2.1 Dirichlet and Neumann boundary conditions

In order to collect some notation we shall use later, let us first consider special choices of the boundary conditions (5.2).

The Neumann Laplacian $-\Delta_N$ on $\mathcal{H}$ acts as the second derivative operator (5.1) equipped with the operator domain $\mathsf{D}(-\Delta_N)$ consisting of functions ψ from $W^{2,2}(-a,a)$ that satisfy (5.2) with $c_\pm = 0$. The Dirichlet Laplacian $-\Delta_D$ on $\mathcal{H}$ can be considered as the other extreme case by formally putting $c_\pm = +\infty$; it is properly defined as the second derivative operator (5.1) with the operator domain $\mathsf{D}(-\Delta_D) := W^{2,2}(-a,a) \cap W_0^{1,2}(-a,a)$. Both $-\Delta_N$ and $-\Delta_D$ are self-adjoint operators with compact resolvent.

The spectrum of the Dirichlet and Neumann Laplacians in our one-dimensional situation is well known:

$$\begin{aligned} \sigma(-\Delta_D) &= \{k_n^2\}_{n=1}^\infty\,, \\ \sigma(-\Delta_N) &= \{k_n^2\}_{n=0}^\infty\,, \end{aligned} \qquad \text{with} \qquad k_n := \frac{n\pi}{2a}\,.$$

The corresponding eigenfunctions are respectively given by

$$\chi_n^D(x) := \frac{1}{\sqrt{a}} \sin k_n(x+a), \qquad \chi_n^N(x) := \begin{cases} \frac{1}{\sqrt{2a}} & \text{if } n=0\,, \\ \frac{1}{\sqrt{a}} \cos k_n(x+a) & \text{if } n \geq 1\,. \end{cases} \tag{5.4}$$

To simplify some expressions in the sequel, we extend the notation by $\chi_0^D := 0$.

Next we introduce a "momentum" operator p and its adjoint p^*:

$$\begin{aligned} p\psi &:= -\mathrm{i}\psi', & p^*\psi &= -\mathrm{i}\psi', \\ \mathsf{D}(p) &:= W_0^{1,2}(-a,a), & \mathsf{D}(p^*) &= W^{1,2}(-a,a). \end{aligned} \tag{5.5}$$

The following identities hold:

$$\begin{aligned} \mathrm{i}p\chi_n^D &= k_n\chi_n^N, & \mathrm{i}p^*\chi_n^N &= -k_n\chi_n^D, \\ -\Delta_D &= p^*p, & -\Delta_N &= pp^*. \end{aligned} \tag{5.6}$$

The resolvents $(-\Delta_D - k^2)^{-1}$, $(-\Delta_N - k^2)^{-1}$ act as integral operators with simple kernels (Green's functions) $\mathcal{G}_D^k$ and $\mathcal{G}_N^k$, respectively:

$$\begin{aligned} \mathcal{G}_D^k(x,y) &= \frac{-\sin(k(x+a))\,\sin(k(y-a))}{k\,\sin(2ka)}\,, \quad x<y\,, \\ \mathcal{G}_N^k(x,y) &= \frac{-\cos(k(x+a))\,\cos(k(y-a))}{k\,\sin(2ka)}\,, \quad x<y\,, \end{aligned} \tag{5.7}$$

with x,y exchanged for $x>y$. Here k^2 is supposed to belong to the resolvent set of the respective operator.

For $k=0$, the kernel of $(-\Delta_D)^{-1}$ simplifies to

$$\mathcal{G}_D^0(x,y) = \frac{(x+a)(a-y)}{2a}\,, \quad x<y\,, \tag{5.8}$$

with x,y exchanged for $x>y$. The resolvent of $-\Delta_N$ does not exist for $k=0$, of course, but one can still introduce the reduced resolvent $\left(-\Delta_N^{\perp}\right)^{-1}$ of the Neumann Laplacian with respect to the eigenvalue 0 (see [26, Sec. III.6.5] for the concept of reduced resolvent). From the point of view of the spectral theorem:

$$\left(-\Delta_N^{\perp}\right)^{-1} = \sum_{n=1}^{\infty} \frac{1}{k_n^2}\,\chi_n^N\langle\chi_n^N,\cdot\rangle. \tag{5.9}$$

The corresponding integral kernel $\mathcal{G}_N^{\perp}(x,y)$ can be obtained by taking the limit $k\to 0$ of the regularized expression $G_N^k(x,y) + k^{-2}\chi_0^N(x)\chi_0^N(y)$. We find

$$\mathcal{G}_N^{\perp}(x,y) = \frac{(x+a)^2}{4a} + \frac{(y-a)^2}{4a} - \frac{a}{3}\,, \quad x<y\,, \tag{5.10}$$

with x,y exchanged for $x>y$.

Finally, we introduce operators

$$J^{\iota} := \sum_{n=0}^{\infty} C_n^2\,\chi_n^{\iota}\langle\chi_n^{\iota},\cdot\rangle\,, \qquad \iota\in\{D,N\}\,, \tag{5.11}$$

where C_n are positive numbers satisfying

$$0 < m_1 < C_n < m_2 < \infty \tag{5.12}$$

for all $n\geq 0$, with given positive m_1, m_2. The sum in the definition (5.11), as well as all other analogous expressions in the following, are understood as limits in the strong sense.

5.2.2 General properties of H

We give a precise meaning to (5.1)–(5.2) via an operator realization H on the Hilbert space $\mathcal{H}\equiv L^2(-a,a)$ defined by

$$\begin{aligned} H\psi &:= -\psi'', \\ \mathsf{D}(H) &:= \left\{\psi\in W^{2,2}(-a,a):\ \psi'(\pm a) + c_{\pm}\psi(\pm a) = 0\right\}. \end{aligned} \tag{5.13}$$

It is customarily introduced as the m-sectorial operator associated with the densely defined, closed, sectorial quadratic form

$$\begin{aligned} t_H[\psi] &:= \|\psi'\|^2 + c_+|\psi(a)|^2 - c_-|\psi(-a)|^2, \\ \mathsf{D}(t_H) &:= W^{1,2}(-a,a), \end{aligned} \tag{5.14}$$

by the representation theorem [26, Sec. VI.2.1]. Here $\|\cdot\|$ denotes the standard norm in $\mathcal{H}$; the corresponding inner product will be denoted by $\langle\cdot,\cdot\rangle$ and it will be assumed to be antilinear in the first component.

Proposition 5.1 (General known facts)**.**

(i) *H is m-sectorial. The adjoint operator H^* is obtained by taking the complex conjugation of $c_\pm$ in the boundary conditions* (5.2)*.*

(ii) *H forms a holomorphic family of operators of type (B) with respect to the boundary parameters $c_\pm$.*

(iii) *H has compact resolvent.*

(iv) *H is a discrete spectral operator.*

(v) *If all eigenvalues are simple, then H is similar to a normal operator. If the spectrum of H is in addition real, then H is similar to a self-adjoint operator.*

For properties (i)–(iii) we refer to the book of Kato [26] (see, in particular, Ex. VI.2.16 and Thm. VI.2.5, Ex. VII.4.11, and Thm. VII.4.3, respectively). The proof of (iv) is contained in Chapt. XIX.3 of the monograph of Dunford and Schwartz [13]. Property (v) is a consequence of (iv). The similarity to a normal operator can be equivalently stated as the Riesz basicity of the eigenvectors of H; this property is shared by all second derivative operators with strongly regular boundary conditions [36].

Although the eigenvalues of H are generically simple, degeneracies may appear. However, the only possibility are the eigenvalues of algebraic multiplicity two and geometric multiplicity one. In this case, operator H cannot be similar to a normal one, nevertheless, the eigenvectors together with generalized eigenvectors still form a Riesz basis.

Now we turn to symmetry properties of H.

Definition 5.1 ($\mathcal{PT}$-symmetry)**.** We say that H is $\mathcal{PT}$-symmetric if

$$[\mathcal{PT}, H] = 0, \tag{5.15}$$

where $\mathcal{P}$ and $\mathcal{T}$ are the bounded (respectively linear and antilinear) operators defined on the whole Hilbert space $\mathcal{H}$ by

$$(\mathcal{P}\psi)(x) := \psi(-x), \quad (\mathcal{T}\psi)(x) := \overline{\psi(x)}. \tag{5.16}$$

It should be stressed that $\mathcal{PT}$ is an antilinear operator. The commutator relation (5.15) means precisely that

$$(\mathcal{PT})H \subset H(\mathcal{PT}),$$

as usual for the commutativity of an unbounded operator with a bounded one (*cf* [26, Sec. III.5.6]). In the quantum-mechanical context, $\mathcal{P}$ corresponds to the parity inversion (space reflection), while $\mathcal{T}$ is the time reversal operator.

Definition 5.2 (S-self-adjointness)**.** We say that H is S-self-adjoint if the relation $H = S^{-1}H^*S$ holds with a boundedly invertible operator S.

We will use this concept in a wide sense, with S being either linear or antilinear operator. If S is a conjugation operator (*i.e.* antilinear involution), then our definition coincides with the concept of J-self-adjointness [14, Sec. III.5].

While Definition 5.2 is quite general, Definition 5.1 makes sense for operators in a complex functional Hilbert space only. In our case, we have:

Proposition 5.2 (Symmetry properties)**.**

(i) *H is $\mathcal{T}$-self-adjoint.*

(ii) *H is $\mathcal{P}$-self-adjoint if, and only if, $c_- = -\overline{c_+}$.*

(iii) *H is $\mathcal{PT}$-symmetric if, and only if, $c_- = -\overline{c_+}$.*

Property (ii) coincides with the notion of self-adjointness in the Krein space equipped with the indefinite inner product $\langle\cdot, \mathcal{P}\cdot\rangle$. It is also referred to as $\mathcal{P}$-pseudo-Hermiticity in physical literature (see, *e.g.*, [37]). In our case, it follows from Proposition 5.2 that H is $\mathcal{P}$-self-adjoint if, and only if, H is $\mathcal{PT}$-symmetric. In general, however, these two notions are unrelated (for a class of $\mathcal{PT}$-symmetric operators which are not $\mathcal{P}$-self-adjoint, see *e.g.* [31, Rem.4.10]).

It follows from Proposition 5.2.(i) that the residual spectrum of H is empty (*cf* [8, Corol. 2.1]). Alternatively, it is a consequence of Proposition 5.1.(iii), which in addition implies that the spectrum of H is purely discrete.

We denote the (countable) set of eigenvalues of H by $\{\lambda_n\}_{n=0}^{\infty}$ and the corresponding set of eigenfunctions by $\{\psi_n\}_{n=0}^{\infty}$. Similarly, let $\{\overline{\lambda_n}\}_{n=0}^{\infty}$ and $\{\phi_n\}_{n=0}^{\infty}$ be the set of eigenvalues and eigenfunctions of the adjoint operator H^*. That is

$$H\psi_n = \lambda_n \psi_n, \qquad H^*\phi_n = \overline{\lambda_n}\phi_n. \tag{5.17}$$

Eigenfunctions ψ_n and ϕ_m corresponding to different eigenvalues, *i.e.* $\lambda_n \neq \lambda_m$, are clearly orthogonal. Solving the eigenvalue equation for H in terms of sine and cosine functions, it is straightforward to reduce the boundary value problem to an algebraic one.

Proposition 5.3 (Spectrum)**.** *The eigenvalues $\lambda_n = l_n^2$ of H are solutions of the implicit equation*

$$\sin(2al)(c_-c_+ + l^2) + (c_- - c_+)l\cos(2al) = 0\,. \tag{5.18}$$

The corresponding eigenfunctions of H and H^* respectively read

$$\begin{aligned}\psi_n(x) &= A_n\frac{1}{\sqrt{a}}\left(\cos(l_n(x+a)) - \frac{c_-}{l_n}\sin(l_n(x+a))\right),\\ \phi_n(x) &= \frac{1}{\sqrt{a}}\left(\cos(\overline{l_n}(x+a)) - \frac{\overline{c_-}}{\overline{l_n}}\sin(\overline{l_n}(x+a))\right).\end{aligned} \tag{5.19}$$

If all eigenvalues are simple, ψ_n can be normalized through the coefficients A_n in such a way that $\langle\psi_n,\phi_m\rangle = \delta_{nm}$.

The spectrum of H has been described more explicitly for the $\mathcal{PT}$-symmetric case. First of all, as a consequence of the symmetry, we know that the spectrum is symmetric with respect to the real axis. In the following proposition we summarize more precise results obtained in [30, 31].

Proposition 5.4 ($\mathcal{PT}$-symmetric spectrum)**.** *Let $c_\pm = \mathrm{i}\alpha \pm \beta$, with $\alpha, \beta \in \mathbb{R}$.*

1. *If $\beta = 0$ then all eigenvalues of H are real,*

$$\lambda_0 = \alpha^2, \quad \lambda_n = k_n^2, \quad n \in \mathbb{N}. \tag{5.20}$$

The corresponding eigenfunctions of H and H^* respectively read

$$\begin{aligned}\psi_0(x) &= A_0 e^{-\mathrm{i}\alpha(x+a)}, \quad \psi_n(x) = A_n\left(\chi_n^N(x) - \mathrm{i}\frac{\alpha}{k_n}\chi_n^D(x)\right),\\ \phi_0(x) &= \frac{1}{\sqrt{2a}}e^{\mathrm{i}\alpha(x+a)}, \quad \phi_n(x) = \chi_n^N(x) + \mathrm{i}\frac{\alpha}{k_n}\chi_n^D(x).\end{aligned} \tag{5.21}$$

If $\alpha \neq k_n$ for every $n \in \mathbb{N}$, then all the eigenvalues are simple and choosing

$$A_0 := \frac{\alpha e^{2\mathrm{i}\alpha a}\sqrt{2a}}{\sin(2\alpha a)}, \quad A_n := \frac{k_n^2}{k_n^2 - \alpha^2}, \tag{5.22}$$

we have the biorthonormal relations $\langle\psi_n,\phi_m\rangle = \delta_{nm}$.

2. *If $\beta > 0$, then all the eigenvalues of H are real and simple.*

3. *If $\beta < 0$, then all the eigenvalues are either real or there is one pair of complex conjugated eigenvalues with real part located in the neighbourhood of $\alpha^2 + \beta^2$.*

In any case, the eigenvalue equation (5.18) *can be rewritten as*

$$(l^2 - \alpha^2 - \beta^2)\sin(2al) - 2\beta l\cos(2al) = 0. \tag{5.23}$$

5.2.3 Concept of the metric operator

We recall the concept of metric operator (or quasi-Hermitian operators introduced in [11]), widely used in $\mathcal{PT}$-symmetric literature.

Definition 5.3 (Metric operator and quasi-Hermiticity)**.** Bounded positive [1] operator Θ with bounded inverse is called a metric operator for H, if H is Θ-self-adjoint. H is then called quasi-Hermitian.

[1] A is positive if $\langle f, Af\rangle > 0$ for all $f \in \mathcal{H}$, $f \neq 0$.

It is obvious that the quasi-Hermitian operator H is self-adjoint with respect to the modified inner product $\langle\cdot,\cdot\rangle_\Theta := \langle\cdot,\Theta\cdot\rangle$. It is also not difficult to show that the metric operator exists if, and only if, H is similar to a self-adjoint operator. Moreover, since H has purely discrete spectrum, the metric operator can be obtained as

$$\Theta = \sum_{n=0}^{\infty} C_n^2\, \phi_n \langle \phi_n, \cdot\rangle, \tag{5.24}$$

where ϕ_n are eigenfunctions of H^* and C_n are real constants satisfying (5.12). As mentioned below (5.11), the sum is understood as a limit in the strong sense.

The expression (5.24) illustrates a non-uniqueness of the metric operator caused by the arbitrariness of C_n. The latter can be actually viewed as a modification of the normalization of functions ϕ_n. Choosing different sequences $\{C_n\}_{n=0}^{\infty}$, we obtain all metric operators for H, *cf* [42, 44].

It is important to stress that if we define an operator Θ by (5.24), we find that such Θ is bounded, positive, and with bounded inverse whenever $\{\phi_n\}_{n=0}^{\infty}$ is a Riesz basis. Thus, by virtue of Proposition 5.1.(v), such a Θ exists if, and only if, all eigenvalues of H are simple. However, the Θ-self-adjointness of H is satisfied if, and only if, the spectrum of H is real. Otherwise, only $\Theta H \Theta^{-1} H^* = H^* \Theta H \Theta^{-1}$ holds, *cf* [44], which is equivalent to the fact that H is similar to a normal operator.

In the following, the operator Θ is always defined by (5.24) regardless if it is a metric operator for H in view of Definition 5.3.

It should be also noted that Θ, as a positive operator, can be always decomposed to

$$\Theta = \Omega^*\Omega. \tag{5.25}$$

One example of such Ω is obviously $\sqrt{\Theta}$. We shall take the advantage of some different decompositions of the type (5.25) later.

It follows easily from Definition 5.3 that the operator h defined by (5.3) with Ω given by (5.25) is self-adjoint if Θ is a metric operator for H. If all eigenvalues of H are simple but no longer entirely real, h is (only) a normal operator. Conversely, if (5.3) holds with a self-adjoint h, then it is easily seen that (5.25) represents a metric for H. We summarize the considerations into the following proposition.

Proposition 5.5. *H is quasi-Hermitian if, and only if, H is similar to a self-adjoint operator.*

5.2.4 Concept of the $\mathcal{C}$ operator

For $\mathcal{PT}$-symmetric operators, the notion of $\mathcal{C}$ operator was introduced in [7] and formalized in [2]. It was observed in [34] and in many works after that paper that Krein spaces provide suitable framework for studying $\mathcal{PT}$-symmetric operators. Indeed, $\mathcal{PT}$-symmetric operators which are at the same time $\mathcal{P}$-self-adjoint are in fact self-adjoint in the Krein space equipped with the indefinite inner product $\langle\cdot,\mathcal{P}\cdot\rangle$. Recall that our operator H is $\mathcal{P}$-self-adjoint if, and only if, it is $\mathcal{PT}$-symmetric (*cf* Proposition 5.2).

Definition 5.4 ($\mathcal{C}$ operator)**.** Assume that H is $\mathcal{P}$-self-adjoint (*cf* Proposition 5.2). We say that H possesses the property of $\mathcal{C}$-symmetry, if there exists a bounded linear operator $\mathcal{C}$ such that $[H,\mathcal{C}]=0$, $\mathcal{C}^2 = I$, and $\mathcal{PC}$ is a metric operator for H.

Thus, from the point of view of metric operators, we can find the $\mathcal{C}$ operator as $\mathcal{C} := \mathcal{P}\Theta$ for Θ satisfying $(\mathcal{P}\Theta)^2 = I$. Hence $\mathcal{C}$-symmetry allows us to naturally choose a metric operator. Besides a possible physical interpretation of $\mathcal{C}$ discussed in [6, 5], it appears naturally in the Krein spaces framework as pointed out in [32, 33] as a fundamental symmetry of the Krein space $(\mathcal{H},\langle\cdot,\mathcal{P}\cdot\rangle)$ with an underlying Hilbert space $(\mathcal{H},\langle\cdot,\mathcal{PC}\cdot\rangle)$.

5.3 General results

In this section we provide general properties of the metric operator Θ defined in (5.24) and its decompositions Ω from (5.25). Further, we investigate the operator h defined in (5.3) and its quadratic form.

5.3.1 The similarity transformation

Let $\{\psi_n\}_{n=0}^{\infty}$ and $\{\phi_n\}_{n=0}^{\infty}$ denote the set of eigenvectors of H and H^*, respectively. We assume that ψ_n and ϕ_n form Riesz bases and that they are normalized in such a way that $\langle\psi_n,\phi_m\rangle = \delta_{mn}$. In view of Propositions 5.1, 5.3, we know that this is satisfied if all the eigenvalues of H are simple, which is a generic situation.

Let $\{e_n\}_{n=0}^{\infty}$ be any orthonormal basis of $\mathcal{H}$. If all eigenvalues of H are simple, we introduce an operator Ω by

$$\Omega := \sum_{n=0}^{\infty} e_n \langle \phi_n, \cdot \rangle. \tag{5.26}$$

Clearly, $\Omega : \psi_n \mapsto e_n$.

Ω is defined only if all eigenvalues are simple, however, sometimes it is possible to extend it by continuity, see examples in Section 5.4. Nonetheless, such Ω is typically not invertible and the dimension of the kernel corresponds to the size of Jordan blocks appearing in the spectrum of H.

Basic properties of Ω are summarized in the following.

Lemma 5.1. *Let all eigenvalues of H be simple. Then Ω is a bounded operator with bounded inverse given by*

$$\Omega^{-1} = \sum_{n=0}^{\infty} \psi_n \langle e_n, \cdot \rangle, \tag{5.27}$$

i.e. $\Omega^{-1} : e_n \mapsto \psi_n$. *The adjoint of Ω reads*

$$\Omega^* = \sum_{n=0}^{\infty} \phi_n \langle e_n, \cdot \rangle. \tag{5.28}$$

i.e. $\Omega^* : e_n \mapsto \phi_n$ *and* $\Omega^*\Omega = \Theta$, *where Θ is defined in* (5.24) *with* $C_n = 1$.

Furthermore, we show how the operator Ω can be realized.

Theorem 5.1. *Let all eigenvalues of H be simple. Ω can be expressed as*

$$\Omega = U + L, \tag{5.29}$$

where $U := \sum_{n=0}^{\infty} e_n \langle \chi_n^N, \cdot \rangle$, i.e. $U : \chi_n^N \mapsto e_n$, *is a unitary operator, and L is a Hilbert-Schmidt operator.*

Proof. At first we remark that it suffices to prove that $\Omega = I + \tilde{L}$ for $e_n := \chi_n^N$, where $\tilde{L}$ is Hilbert-Schmidt. More precisely, if we compose U from the claim and $I+\tilde{L}$, we obtain Ω in (5.29) since $L = U\tilde{L}$ is Hilbert-Schmidt too. Thus, we consider this choice of e_n in the following. Furthermore, we put $a := \pi/2$ for simplification of the formulae. This specific choice is in fact harmless, since we can easily transfer the results for different a using the isometry $V : L^2(-\pi/2, \pi/2) \to L^2(-a, a)$ defined by $\psi(x) \mapsto \sqrt{\frac{\pi}{2a}}\psi(\frac{\pi x}{2a})$.

The asymptotic analysis of eigenvalues of H in [13, proof of Lem. XIX.3.10] shows that

$$\begin{aligned} l_n &= n + \frac{c_+ - c_-}{\pi n} + \mathcal{O}(n^{-2}), \\ \lambda_n \equiv l_n^2 &= k_n^2 + \frac{2(c_+ - c_-)}{\pi} + \mathcal{O}(n^{-1}), \end{aligned} \tag{5.30}$$

and $|\Im(l_n)|$ is uniformly bounded in n. These formulae are valid except for a finite number N_0 of eigenvalues.

We set $\varepsilon_n := l_n - k_n = l_n - n$. Using elementary trigonometric identities, we rewrite the eigenfunctions ϕ_n as follows

$$\begin{aligned} \phi_n(x) = {} & \chi_n^N(x) \cos\left(\overline{\varepsilon_n}(x+a)\right) - \chi_n^D(x) \sin\left(\overline{\varepsilon_n}(x+a)\right) \\ & - \frac{\overline{c_-}}{\overline{l_n}} \left[\chi_n^D(x) \cos(\overline{\varepsilon_n}(x+a)) + \chi_n^N(x) \sin\left(\overline{\varepsilon_n}(x+a)\right)\right]. \end{aligned} \tag{5.31}$$

We further rewrite the cosine and sine functions in this expression as

$$\begin{aligned} \cos\left(\overline{\varepsilon_n}(x+a)\right) &= 1 + \overline{\varepsilon_n}^2 \, \frac{\cos\left(\overline{\varepsilon_n}(x+a)\right) - 1}{\overline{\varepsilon_n}^2} =: 1 + \overline{\varepsilon_n}^2 \, c_n(x), \\ \sin\left(\overline{\varepsilon_n}(x+a)\right) &= \overline{\varepsilon_n} \, \frac{\sin\left(\overline{\varepsilon_n}(x+a)\right)}{\overline{\varepsilon_n}} =: \overline{\varepsilon_n} \, s_n(x). \end{aligned} \tag{5.32}$$

Note that $\|c_n\|$ and $\|s_n\|$ are uniformly bounded in n because of the properties of ε_n. The building block $\chi_n^N \langle \phi_n, \cdot \rangle$ of Ω then becomes

$$\begin{aligned} \chi_n^N \langle \phi_n, \cdot \rangle = {} & \chi_n^N \langle \chi_n^N, \cdot \rangle + \varepsilon_n^2 \chi_n^N \langle \chi_n^N c_n, \cdot \rangle - \varepsilon_n \chi_n^N \langle \chi_n^D s_n, \cdot \rangle \\ & - \frac{c_-}{l_n} \left(\chi_n^N \langle \chi_n^D, \cdot \rangle + \varepsilon_n^2 \chi_n^N \langle \chi_n^D c_n, \cdot \rangle + \varepsilon_n \chi_n^N \langle \chi_n^N s_n, \cdot \rangle\right). \end{aligned} \tag{5.33}$$

Taking the sum of $\chi_n^N \langle \phi_n, \cdot \rangle$ as in (5.26), we obviously get $\Omega = I + \tilde{L}$.

It remains to show that the Hilbert-Schmidt norm $\|\tilde{L}\|_{\mathrm{HS}}$ of $\tilde{L}$ is finite. We will understand $\tilde{L}$ as a sum $\tilde{L} = \tilde{L}_{N_0} + \tilde{L}_\infty$, where

$$\tilde{L}_{N_0} := \sum_{n=0}^{N_0-1} \chi_n^N \langle \tilde{\phi}_n, \cdot \rangle, \quad \tilde{L}_\infty := \sum_{n=N_0}^{\infty} \chi_n^N \langle \tilde{\phi}_n, \cdot \rangle, \tag{5.34}$$

and $\tilde{\phi}_n := \phi_n - \chi_n^N$. $\tilde{L}_{N_0}$ is a finite rank operator, hence it is automatically Hilbert-Schmidt and it suffices to consider $\tilde{L}_\infty$ in the rest of the proof. We estimate explicitly only one term in the expression for $\|\tilde{L}_\infty\|_{\mathrm{HS}}^2$, the rest follows in a similar way:

$$\begin{aligned} &\sum_{p=0}^{\infty} \left\langle \sum_{n=N_0}^{\infty} \varepsilon_n \chi_n^N \left\langle \chi_n^D s_n, \chi_p^N \right\rangle, \sum_{m=N_0}^{\infty} \varepsilon_m \chi_m^N \left\langle \chi_m^D s_m, \chi_p^N \right\rangle \right\rangle \\ &= \sum_{p=0}^{\infty} \sum_{n=N_0}^{\infty} |\varepsilon_n|^2 \left| \left\langle \chi_n^D s_n, \chi_p^N \right\rangle \right|^2 \leq \frac{1}{a} \sum_{n=N_0}^{\infty} |\varepsilon_n|^2 \|s_n\|^2 < \infty. \end{aligned} \tag{5.35}$$

Here the first inequality follows by the Bessel inequality (after interchanging the order of summation, which is justified) and by estimating χ_n^D by its supremum norm. The asymptotic behaviour of ε_n and the uniform boundedness of $\|s_n\|$ are used in the last step. □

Remark 5.1. The proof can be little shortened using the notion of Bari basis [17, Ch.VI]. Indeed, combining Thm. VI.3.3 from [17] (or the results of the original work [28]) with the asymptotics (5.30), it can be verified in the analogous way as in the proof above that eigenfunctions of H form the Bari basis, so that the results follow. This also suggests that Theorem 3.2 might be well known in some respect, however, unable to find a suitable reference and in order to make the present paper self-contained, we present the entire, direct proof here. This remark applies also to Theorem 5.4.

Corollary 5.1. *Let all eigenvalues of H be simple. Then*

$$\Theta := \Omega^* \Omega = I + K \tag{5.36}$$

coincides with Θ defined in (5.24) with $C_n = 1$. Here K is a Hilbert-Schmidt operator that can be realized as an integral operator with a kernel belonging to $L^2((-a,a) \times (-a,a))$.

Proof. The claim follows from Theorem 5.1 and the well-known facts that Hilbert-Schmidt operators are *-both-sided ideal in the space of bounded operators and can be realized as integral ones, see [39, Thm.VI.23]. □

Remark 5.2. Slight modification of the definition of Ω and the proof of Theorem 5.1 yields the analogous result for operators Θ defined in (5.24) with arbitrary C_n. It suffices to consider $f_n := C_n e_n$ instead of e_n. The resulting form is

$$\Theta = J^N + \tilde{K}, \tag{5.37}$$

where J^N is defined in (5.11) and $\tilde{K}$ is again a Hilbert-Schmidt operator. J^N itself, however, can be a sum of a bounded and a Hilbert-Schmidt operator, as we shall see in examples.

5.3.2 The operator h similar to H

We further investigate the properties of the operator h from (5.3) and its quadratic form.

Proposition 5.6. *Let $\mathcal{S}$ be an open connected set in $\mathbb{C}^2$ such that for all $(c_-, c_+) \in \mathcal{S}$ all eigenvalues of H are simple. Then Ω and thereby Θ are bounded holomorphic families in $\mathcal{S}$ with respect to parameters $c_\pm$.*

Proof. We verify the criterion stated in [26, Sec. VII.1.1]. We have proved already that Ω is bounded. It remains to show that $\langle f, \Omega g \rangle$ is holomorphic for every f, g from a fundamental set of $\mathcal{H}$ that we choose as the orthonormal basis $\{e_n\}_{n=0}^\infty$. $\langle e_m, \Omega e_n \rangle = \langle \phi_m, e_n \rangle$ is holomorphic because ϕ_m is an eigenfunction of the operator H^*, which can be viewed as a holomorphic family of operators of type (B) with respect to the parameters $c_\pm$. □

Corollary 5.2. *Assume the hypothesis of Proposition 5.6. Then $h := \Omega H \Omega^{-1}$ is a holomorphic family of operators in $\mathcal{S}$ with respect to parameters $c_\pm$.*

Since the operator H is a holomorphic family of type (B), *i.e.* it is naturally defined via quadratic forms with the domain $W^{1,2}(-a,a)$ independent of the parameters $c_\pm$, h is expected to possess a similar property. To prove it, we have to particularly show that the associated quadratic forms corresponding to different values of $c_\pm$ have the same domain, which is not guaranteed by Corollary 5.2. To this end we analyse the quadratic form associated to h, where we set $e_n := \chi_n^N$ in the definition of Ω.

Theorem 5.2. *Let all eigenvalues of H be simple and let $e_n := \chi_n^N$ in (5.26). Then $\Omega = I+L$ and $\Omega^{-1} = I+M$, where L, M are Hilbert-Schmidt operators. $\Omega, \Omega^*, \Omega^{-1}, (\Omega^{-1})^*$ are bounded operators on $W^{1,2}(-a,a)$ and $W^{2,2}(-a,a)$. Furthermore, the following estimates hold for all $\phi \in W^{1,2}(-a,a)$ and arbitrary $\delta > 0$:*

$$\begin{aligned} \|(L^*\phi)'\|^2 &\le C\left(\delta\,\|\phi'\|^2 + \delta^{-2}\|\phi\|^2\right), \\ \|(M\phi)'\|^2 &\le C\left(\delta\,\|\phi'\|^2 + \delta^{-2}\|\phi\|^2\right), \end{aligned} \tag{5.38}$$

with C being constants not dependent on δ and ϕ.

Proof. We set $a := \pi/2$ as in the proof of Theorem 5.1. M is Hilbert-Schmidt since $I = \Omega\Omega^{-1} = I+L+M+LM$ and L is Hilbert-Schmidt.

We consider Ω^* at first. Following the proof of Theorem 5.1, L^* can be written as

$$L^* f = \sum_{k=0}^{\infty} \tilde{\phi}_k \langle \chi_k^N, f\rangle, \tag{5.39}$$

where $\tilde{\phi}_k := \phi_k - \chi_k^N$ and $f \in \mathcal{H}$. We show that L^* is bounded on $W^{1,2}(-a,a)$. We estimate the Hilbert-Schmidt norm of L^* on $W^{1,2}(-a,a)$ with help of the orthonormal basis $f_n := \chi_n^N/\sqrt{1+n^2}$. In fact, it suffices to estimate:

$$\sum_{n=0}^{\infty} \langle (L^* f_n)', (L^* f_n)'\rangle = \sum_{n=0}^{\infty} \frac{1}{1+n^2}\|\tilde{\phi}_n'\|^2 \tag{5.40}$$

where (recall (5.31) and (5.32))

$$\begin{aligned} \tilde{\phi}_n' = &-n\overline{\varepsilon_n}^2\,\chi_n^D c_n - \overline{\varepsilon_n}^2\,\chi_n^N s_n - n\overline{\varepsilon_n}\,\chi_n^N s_n - \overline{\varepsilon_n}\,\chi_n^D(1+\overline{\varepsilon_n}^2\,c_n) \\ &+ \overline{c_-}\left[\chi_n^N(1+\overline{\varepsilon_n}^2\,c_n) - \overline{\varepsilon_n}\,\chi_n^D s_n\right]. \end{aligned} \tag{5.41}$$

Using the asymptotic properties of ε_n and the uniform boundedness of c_n, s_n (see (5.30) and (5.32), respectively) together with the normalization of χ_n^ι, we conclude that $\|\tilde{\phi}_n'\| \le C$ uniformly in n. Therefore (5.40) is finite.

Using the same technique, we can show that the Hilbert-Schmidt norm of L^* in $W^{2,2}(-a,a)$ is finite. To this end we select the basis $\chi_n^N/\sqrt{1+n^2+n^4}$, the rest is based on $\|\tilde{\phi}_n''\| = \mathcal{O}(n)$ as $n \to \infty$.

Let us now establish the inequalities (5.38). Consider $\phi \in W^{1,2}(-a,a)$, its basis decomposition $\phi = \sum_{n=0}^\infty \alpha_n \chi_n^N$, and the identity

$$\sum_{n=0}^{\infty} |n\alpha_n|^2 = \|\phi'\|^2. \tag{5.42}$$

Hence,

$$\|(L^*\phi)'\|^2 = \sum_{m,n=0}^{\infty} \overline{\alpha_m}\alpha_n \langle \tilde{\phi}_m', \tilde{\phi}_n'\rangle, \tag{5.43}$$

and having the explicit form of $\tilde{\phi}_n'$, see (5.41), we have to estimate several terms. We show the technique only for one term, the estimate of remaining terms is analogous. First, using the uniform boundedness of $\|c_n\|, \|s_n\|$, the asymptotics $\varepsilon_n = \mathcal{O}(n^{-1})$ and the uniform boundedness of $\|\chi_n^N\|_\infty$, it is easy to see that

$$\sum_{m,n=0}^{\infty} m\,n\,|\alpha_m||\alpha_n||\varepsilon_m||\varepsilon_n||\langle \chi_m^N s_m, \chi_n^N s_n\rangle| \le C\left(\sum_{n=1}^{\infty}|\alpha_n|\right)^2$$

holds with some positive constant C. It remains to estimate the l^1-norm of α_n by the l^2-norms of α_n and $n\alpha_n$ (which equal $\|\phi\|$ and $\|\phi'\|$, respectively). This is rather algebraic:

$$\begin{aligned} \left(\sum_{n=1}^{\infty}|\alpha_n|\right)^2 &= \left(\sum_{n=1}^{\infty}\left(|\alpha_n|\,n\right)^b|\alpha_n|^{1-b}\,n^{-b}\right)^2 \\ &\le \left(\sum_{n=1}^{\infty}|\alpha_n|^2\,n^2\right)^b\left(\sum_{n=1}^{\infty}|\alpha_n|^2\right)^{1-b}\left(\sum_{n=1}^{\infty}n^{-2b}\right) \\ &\le C_b\,\|\phi'\|^{2b}\,\|\phi\|^{2(1-b)} \\ &\le C_b\left(b\,\delta\,\|\phi'\|^2 + (1-b)\,\delta^{-\frac{b}{1-b}}\,\|\phi\|^2\right), \end{aligned}$$

with any $b, \delta \in (0,1)$. Here the first inequality follows by the generalized Hölder inequality and the last one is a consequence of the Young inequality. The exponent b is chosen in such a way that $2b > 1$, so that the sum of n^{-2b} (denoted by C_b) converges. If we put $b = 2/3$, we obtain the inequality in the claim.

One can show, using the asymptotics (5.30), that it follows from the normalization requirement $\langle \phi_n, \psi_n \rangle = 1$ that A_n, the normalization constants of ψ_n, see (5.19), satisfy $A_n = 1 + \mathcal{O}(n^{-1})$. Then the claims for Ω^{-1} and M can be derived in the same manner.

To justify that Ω and $(\Omega^{-1})^*$ are bounded on $W^{1,2}(-a,a)$ and $W^{2,2}(-a,a)$, it suffices to realize that Ω^{-1} and Ω^* are invertible because they are invertible in $L^2(-a,a)$ and the inverse is bounded because of the form identity plus compact operator on considered Sobolev spaces. □

Corollary 5.3. *Assume the hypotheses of Theorem 5.2. Then $h := \Omega H \Omega^{-1}$ is a holomorphic family of operators of type (B) with respect to $c_\pm$. The associated quadratic form t_h, in the sense of the representation theorem [26, Thm. VI.2.1], reads*

$$\begin{aligned} t_h[\psi] &= \|\psi'\|^2 + \langle (L^*\psi)', \psi' \rangle + \langle \psi', (M\psi)' \rangle + \langle (L^*\psi)', (M\psi)' \rangle \\ &\quad + c_+ \left[\left(\overline{\psi(a)} + \overline{(L^*\psi)(a)} \right) \left(\psi(a) + (M\psi)(a) \right) \right] \\ &\quad - c_- \left[\left(\overline{\psi(-a)} + \overline{(L^*\psi)(-a)} \right) \left(\psi(-a) + (M\psi)(-a) \right) \right], \\ \mathsf{D}(t_h) &= W^{1,2}(-a,a). \end{aligned} \tag{5.44}$$

Proof. The form t_h defined in (5.44) is sectorial and closed due to the perturbation result [26, Thm. VI.1.33], regarding $u[\psi] := t_h[\psi] - \|\psi'\|^2$ as a perturbation of $t_0[\psi] := \|\psi'\|^2$. Indeed, the inequalities (5.38) applied on $u[\psi]$ yield that u is t_0-bounded with t_0-bound 0. Therefore, due to the first representation theorem [26, Thm. VI.2.1], there is a unique m-sectorial operator associated with t_h. Let us denote it by $\tilde{h}$. Our objective is to show that $\tilde{h} = h$.

Using the definition of h by the similarity transformation, *i.e.* $h = \Omega H \Omega^{-1}$, and the fact that H is associated to t_H, we know that the domain of h are functions u such that, firstly, $\Omega^{-1}u \in W^{1,2}(-a,a)$ and, secondly, there exists $w \in L^2(-a,a)$ such that

$$t_H(\Omega^* v, \Omega^{-1} u) = (v, w) \tag{5.45}$$

for all v such that $\Omega^* v \in W^{1,2}(-a,a)$. However, by Theorem 5.2, Ω, Ω^*, Ω^{-1}, $(\Omega^*)^{-1}$ are bounded on $W^{1,2}(-a,a)$ and it is easy to check that the identity

$$t_H(\Omega^* v, \Omega^{-1} u) = t_h(v, u) \tag{5.46}$$

holds for all $u, v \in W^{1,2}(-a,a)$. Consequently, the operators $\tilde{h}$ and h indeed coincide. □

Remark 5.3. We remark that the boundedness of Ω, Ω^*, Ω^{-1} and $(\Omega^{-1})^*$ in $W^{2,2}(-a,a)$ was not used in the proof Corollary 5.3. Nevertheless, this property is useful if we analyse the domain of h directly from the relation $h = \Omega H \Omega^{-1}$. It follows that $\mathsf{D}(h)$ consists of functions ψ from $W^{2,2}(-a,a)$ satisfying boundary conditions $(\Omega^{-1}\psi)'(\pm a) + c_\pm (\Omega^{-1}\psi)(\pm a) = 0$.

5.4 Closed formulae in $\mathcal{PT}$-symmetric cases

We present closed formulae of operators Θ, Ω and h corresponding to H with special $\mathcal{PT}$-symmetric choice of boundary conditions, $c_\pm := \mathrm{i}\alpha$, with $\alpha \in \mathbb{R}$. This case has already been studied in a similar context in [30, 29], where the first formulae of the metric Θ were given. We substantially generalize these results here.

We essentially rely on the original idea of [29] to “use the spectral theorem backward” to sum up the infinite series appearing in the definition of Θ in (5.24). The attempts to find Ω as the square root of Θ using the holomorphic and self-adjoint calculus are contained in [47, 46], however, only approximations of the resulting self-adjoint operator h similar to H were found there. The main novelty of the present approach comes from the more general factorization (5.25) with (5.26), which enables us to obtain exact results. Formulae contained in this section are obtained by tedious although straightforward calculations that we do not present entirely.

Finally, we present the metric operator for H with general $\mathcal{PT}$-symmetric boundary conditions, $c_\pm := \mathrm{i}\alpha \pm \beta$. In this case, the eigenvalues are no longer explicitly known, nevertheless, the experience from previous examples and formulation of partial differential equation together with a set of “boundary conditions” for the kernel of the integral operator provide the correct result.

5.4.1 Reduction to finding a Neumann metric

Comparing (5.11) with (5.24), we see that J^N and J^D are the metrics for the Neumann and Dirichlet Laplacians, respectively. The former is abbreviated to the "Neumann metric" in the sequel.

We start with the following fundamental result.

Proposition 5.7. *Let* $c_\pm := \mathrm{i}\alpha$, *with* $\alpha \in \mathbb{R}$. *Then the operator* Θ *defined in* (5.24) *has the form*

$$\Theta = J^N + C_0^2\,\theta_1 + J^N\theta_2 + J^D\theta_3, \tag{5.47}$$

where J^ι, *with* $\iota \in \{D, N\}$, *are defined in* (5.11), $C_0 > 0$, *and* θ_i *are integral operators with kernels:*

$$\begin{aligned} \theta_1(x,y) &:= \frac{\mathrm{i}}{a}\, e^{\frac{\mathrm{i}\alpha}{2}(x-y)} \sin\left(\frac{\alpha}{2}(x-y)\right), \\ \theta_2(x,y) &:= \frac{\mathrm{i}\alpha}{2a}\left[y - a\,\mathrm{sgn}(y-x)\right], \\ \theta_3(x,y) &:= \frac{\alpha^2}{2a}\left(a^2 - xy\right) - \frac{\mathrm{i}\alpha}{2a}\,x - \frac{\mathrm{i}\alpha}{2}\left[1 - \mathrm{i}\alpha(y-x)\right]\mathrm{sgn}(y-x). \end{aligned} \tag{5.48}$$

Θ *is the metric operator for* H, *see Definition 5.3, if, and only if,* $\alpha \neq k_n$ *for every* $n \in \mathbb{N}$.

Proof. Using the explicit form (5.21) of functions ϕ_n and the definition (5.24) of Θ, we obtain

$$\begin{aligned} \Theta &= \sum_{n=0}^{\infty} C_n^2 \chi_n^N \langle \chi_n^N, \cdot\rangle + C_0^2\left(\phi_0\langle\phi_0,\cdot\rangle - \chi_0^N\langle\chi_0^N,\cdot\rangle\right) \\ &\quad + \alpha^2 \sum_{n=1}^{\infty} \frac{C_n^2}{k_n^2}\chi_n^D\langle\chi_n^D,\cdot\rangle + \mathrm{i}\alpha\sum_{n=1}^{\infty}\frac{C_n^2}{k_n}\chi_n^D\langle\chi_n^N,\cdot\rangle - \mathrm{i}\alpha\sum_{n=1}^{\infty}\frac{C_n^2}{k_n}\chi_n^N\langle\chi_n^D,\cdot\rangle. \end{aligned} \tag{5.49}$$

Employing the operators J^ι and p, p^* introduced in (5.11) and (5.5), respectively, and relations (5.6) we obtain:

$$\begin{aligned} \Theta &= J^N \sum_{n=0}^{\infty} \chi_n^N\langle\chi_n^N,\cdot\rangle + C_0^2\left(\phi_0\langle\phi_0,\cdot\rangle - \chi_0^N\langle\chi_0^N,\cdot\rangle\right) \\ &\quad + \alpha J^N p \sum_{n=1}^{\infty}\frac{1}{k_n^2}\chi_n^D\langle\chi_n^D,\cdot\rangle \\ &\quad + J^D\left(\alpha^2\sum_{n=1}^{\infty}\frac{1}{k_n^2}\chi_n^D\langle\chi_n^D,\cdot\rangle + \alpha p^*\sum_{n=1}^{\infty}\frac{1}{k_n^2}\chi_n^N\langle\chi_n^N,\cdot\rangle\right). \end{aligned} \tag{5.50}$$

It follows from the functional calculus for self-adjoint operators that (5.50) can be written as

$$\begin{aligned} \Theta = J^N &+ C_0^2\left(\phi_0\langle\phi_0,\cdot\rangle - \chi_0^N\langle\chi_0^N,\cdot\rangle\right) + \alpha J^N p(-\Delta_D)^{-1} \\ &+ J^D\left[\alpha^2(-\Delta_D)^{-1} + \alpha p^*(-\Delta_N^\perp)^{-1}\right]. \end{aligned} \tag{5.51}$$

By inserting the explicit integral kernels of the resolvents, see Section 5.2.1, we obtain the formula (5.47) with (5.48).

To ensure that such Θ represents as metric operator, we recall that the spectrum of H is always real, see Proposition 5.4. Moreover, it is simple if, and only if, the condition in the last claim is satisfied. ☐

Remark 5.4. The formula (5.47) can be rewritten in terms of the operator J^N only. Indeed, it is possible to show that

$$J^D = p^* J^N p(-\Delta_D)^{-1}. \tag{5.52}$$

The final result is then

$$\Theta = J^N + C_0^2\theta_1 + J^N\theta_2 + p^*J^N\theta_4, \tag{5.53}$$

where $\theta_4 := p(-\Delta_D)^{-1}\theta_3$ is an integral operator with kernel

$$\begin{aligned} \theta_4(x,y) = \frac{\alpha}{12a}&\left(y^2(3 - \mathrm{i}\alpha y) + 3x^2(1 - \mathrm{i}\alpha y) + 2a^2\left[1 + \mathrm{i}\alpha(3x - y)\right]\right) \\ &- \frac{1}{4}\alpha\left(2 - \mathrm{i}\alpha(y-x)\right)(y-x)\,\mathrm{sgn}(y-x). \end{aligned} \tag{5.54}$$

Note that the expression (5.54) is a result of a rather lengthy computation.

Any metric operator for H in Proposition 5.7 can be obtained by determining J^N for given constants C_n. Thus we managed to transform the problem of constructing the metric operators for non-self-adjoint operator H to the problem of constructing the metric operators J^N for the Neumann Laplacian $-\Delta_N$. This significantly simplifies the problem, since $-\Delta_N$ is self-adjoint and its metric operators are bounded, positive operators with bounded inverse commuting with $-\Delta_N$. For instance, any bounded, uniformly positive function of $-\Delta_N$ represents a metric operator. Moreover, it was shown in [46] that any J^N can be approximated in the strong sense by a polynomial of $I + \lambda(-\Delta_N - \lambda)^{-1}$, with $\lambda \in \rho(-\Delta_N)$.

We consider two choices of constants C_n in the following and we find final formulae for the corresponding metric operators.

5.4.2 The constant-coefficients metric

Let $C_n^2 := 1$ for every $n \geq 0$. Then $J^N = J^D = I$ and the metric operator Θ reads $\Theta = I + K$, where K is an integral operator with the kernel

$$\begin{aligned}\mathcal{K}(x,y) = \frac{\mathrm{i}}{a}\, e^{\mathrm{i}\frac{\alpha}{2}(x-y)} \sin\left(\frac{\alpha}{2}(x-y)\right) + \frac{\mathrm{i}\alpha}{2a}\left(|y-x| - 2a\right)\operatorname{sgn}(y-x) \\ + \frac{\alpha^2}{2a}\left(a^2 - xy - a|y-x|\right).\end{aligned} \tag{5.55}$$

Formula (5.55) represents a remarkably elegant form for the metric operator found firstly in [30, 29].

5.4.3 The $\mathcal{C}$ operator

Another choice of C_n is motivated by the concept of $\mathcal{C}$ operator, see Definition 5.4. We want to find such Θ that $\mathcal{C}^2 = I$, where $\mathcal{C} = \mathcal{P}\Theta$. Since H is $\mathcal{P}$-self-adjoint, we have $\mathcal{P}\phi_n = D_n\psi_n$ with some numbers D_n. Assuming the non-degeneracy condition $\alpha \neq k_n$ for every $n \geq 0$, an explicit calculation shows that

$$D_0 = \frac{\sin(2\alpha a)}{2\alpha a}, \quad D_n = (-1)^n\, \frac{k_n^2 - \alpha^2}{k_n^2}, \quad n \in \mathbb{N}. \tag{5.56}$$

The condition $(\mathcal{P}\Theta)^2 = I$ then restricts C_n from (5.24) to

$$C_0^2 = \frac{2|\alpha|a}{|\sin(2\alpha a)|}, \quad C_n^2 = \frac{k_n^2}{|k_n^2 - \alpha^2|}, \quad n \in \mathbb{N}. \tag{5.57}$$

In order to simplify the formulae, we consider only $\alpha \in (0, k_1)$ in the following.

Remark 5.5. As mentioned below (5.24), any choice of C_n can be interpreted as a sort of normalisation of ϕ_n. It is therefore interesting to notice that (5.57) results into the symmetric normalization of ϕ_n and ψ_n when $\langle \phi_n, \psi_n \rangle = 1$ is required:

$$\psi_0(x) = \sqrt{\frac{\alpha}{\sin(2\alpha a)}}\, e^{\mathrm{i}\alpha a} e^{-\mathrm{i}\alpha x}, \qquad \psi_n(x) = \frac{k_n}{\sqrt{k_n^2 - \alpha^2}}\left(\chi_n^N(x) - \mathrm{i}\frac{\alpha}{k_n}\chi_n^D(x)\right),$$
$$\phi_0(x) = \sqrt{\frac{\alpha}{\sin(2\alpha a)}}\, e^{\mathrm{i}\alpha a} e^{\mathrm{i}\alpha x}, \qquad \phi_n(x) = \frac{k_n}{\sqrt{k_n^2 - \alpha^2}}\left(\chi_n^N(x) + \mathrm{i}\frac{\alpha}{k_n}\chi_n^D(x)\right).$$

These expressions should be compared with the normalization of (5.21)–(5.22), standardly used in the present paper. The symmetric form of the "present normalization" indicates that the choice (5.57) will lead to a simpler form of Θ than (5.55).

Using (5.57) in the series (5.11), the operators J^ι can be determined by the functional calculus:

$$\begin{aligned}
J^N &= \sum_{n=0}^{\infty} \frac{k_n^2}{k_n^2 - \alpha^2}\, \chi_n^N \langle \chi_n^N, \cdot \rangle + C_0^2\, \chi_0^N \langle \chi_0^N, \cdot \rangle \\
&= (-\Delta_N)(-\Delta_N - \alpha^2)^{-1} + C_0^2\, \chi_0^N \langle \chi_0^N, \cdot \rangle \\
&= I + \alpha^2(-\Delta_N - \alpha^2)^{-1} + C_0^2\, \chi_0^N \langle \chi_0^N, \cdot \rangle, \\
J^D &= \sum_{n=1}^{\infty} \frac{k_n^2}{k_n^2 - \alpha^2}\, \chi_n^D \langle \chi_n^D, \cdot \rangle \\
&= (-\Delta_D)(-\Delta_D - \alpha^2)^{-1} \\
&= I + \alpha^2(-\Delta_D - \alpha^2)^{-1}.
\end{aligned} \tag{5.58}$$

A direct (but very tedious) way how to derive the metric Θ for the choice (5.57) is to express the resolvents of the Dirichlet and Neumann Laplacians from the ultimate expressions in (5.58) by means of the Green's functions (5.7) and compose them with the operators θ_i in (5.47).

However, a more clever way how to proceed is to come back to the operator form (5.51) and perform first some algebraic manipulations with the intermediate expressions appearing in (5.58). First, we clearly have $J^D(-\Delta_D)^{-1} = (-\Delta_D - \alpha^2)^{-1}$. Second, employing (5.5) and the identity $(-\Delta_N)(-\Delta_N^{\perp})^{-1} = I - \chi_0^N \langle \chi_0^N, \cdot \rangle$, we check

$$\left[J^D p^* (-\Delta_N^{\perp})^{-1}\right]^* = p(-\Delta_D - \alpha^2)^{-1}, \quad \left[J^N p(-\Delta_D)^{-1}\right]^* = p^*(-\Delta_N - \alpha^2)^{-1}.$$

Finally, again using (5.5), we verify the intertwining relation $[p(-\Delta_D - \alpha^2)^{-1}]^* = p^*(-\Delta_N - \alpha^2)^{-1}$. Summing up, with our choice (5.57), formula (5.51) simplifies to

$$\begin{aligned}\Theta = I + C_0^2\, \phi_0 \langle \phi_0, \cdot \rangle + \alpha^2(-\Delta_N - \alpha^2)^{-1} + \alpha^2(-\Delta_D - \alpha^2)^{-1} \\ + \alpha\, p(-\Delta_D - \alpha^2)^{-1} + \alpha\, p^*(-\Delta_N - \alpha^2)^{-1}.\end{aligned} \tag{5.59}$$

Now it is easy to substitute (5.7) and after elementary manipulations to conclude with $\Theta = I + K$, where K is an integral operator with the kernel

$$\mathcal{K}(x, y) = \alpha\, e^{-i\alpha(y-x)} \left[\tan(\alpha a) - i\,\mathrm{sgn}(y - x)\right]. \tag{5.60}$$

The operator $\mathcal{C}$ can be found easily by composing $\mathcal{P}$ and Θ. We finally arrive at the formula $\mathcal{C} = \mathcal{P} + L$, where L is an integral operator with the kernel

$$\mathcal{L}(x, y) = \alpha\, e^{-i\alpha(y+x)} \left[\tan(\alpha a) - i\,\mathrm{sgn}(y + x)\right]. \tag{5.61}$$

5.4.4 The self-adjoint operator h similar to H

We present an example of the operator Ω, defined in (5.26) with $e_n := \chi_n^N$, that will be used to find the self-adjoint operator h from (5.3). We recall that the similarity transformation Ω is invertible if all the eigenvalues of H are simple, which is ensured by the condition $\alpha \neq k_n$ for every $n \in \mathbb{N}$. We will actually search for the quadratic form associated to h for which we have the result in Corollary 5.3.

We follow the analogous strategy to obtain formula for Ω as in the proof of Proposition 5.7. The definition of Ω with $e_n := \chi_n^N$ leads to the sum:

$$\begin{aligned}\Omega &= \chi_0^N \langle \phi_0, \cdot \rangle + \sum_{n=1}^{\infty} \chi_n^N \langle \chi_n^N, \cdot \rangle - i\alpha \sum_{n=1}^{\infty} \frac{1}{k_n} \chi_n^N \langle \chi_n^D, \cdot \rangle \\ &= I + \chi_0^N \langle \phi_0, \cdot \rangle - \chi_0^N \langle \chi_0^N, \cdot \rangle + \alpha p \sum_{n=1}^{\infty} \frac{1}{k_n^2} \chi_n^D \langle \chi_n^D, \cdot \rangle \\ &= I + \chi_0^N \langle \phi_0, \cdot \rangle - \chi_0^N \langle \chi_0^N, \cdot \rangle + \alpha p (-\Delta_D)^{-1},\end{aligned} \tag{5.62}$$

where we have used identities (5.6). In the same manner, we obtain the result for the inverse Ω^{-1}:

$$\begin{aligned}\Omega^{-1} &= \psi_0 \langle \chi_0^N, \cdot \rangle + \sum_{n=1}^{\infty} \frac{k_n^2}{k_n^2 - \alpha^2} \chi_n^N \langle \chi_n^N, \cdot \rangle - i\alpha \sum_{n=1}^{\infty} \frac{k_n}{k_n^2 - \alpha^2} \chi_n^D \langle \chi_n^N, \cdot \rangle \\ &= I + \psi_0 \langle \chi_0^N, \cdot \rangle + \alpha^2(-\Delta_N - \alpha^2)^{-1} - \alpha p^*(-\Delta_N - \alpha^2)^{-1}.\end{aligned} \tag{5.63}$$

The operators L, M appearing in the expressions for $\Omega = I + L$ and $\Omega^{-1} = I + M$ are, as expected, integral operators with the kernels $\mathcal{L}$, $\mathcal{M}$ that can be easily obtained using formulae for the Neumann and Dirichlet resolvents (5.7)–(5.8):

$$\begin{aligned}\mathcal{L}(x, y) &= \frac{i\alpha}{2a}\left[y - a\,\mathrm{sgn}(y - x)\right] + \frac{1}{2a}\left(e^{-i\alpha(y+a)} - 1\right), \\ \mathcal{M}(x, y) &= \frac{\alpha e^{i\alpha(a-x)}}{\sin(2\alpha a)} - \frac{\alpha}{2} e^{-i\alpha(x-y)}\left[\cot(2\alpha a) - i\,\mathrm{sgn}(y - x)\right] \\ &\quad - \frac{\alpha e^{-i\alpha(x+y)}}{2\sin(2\alpha a)}.\end{aligned} \tag{5.64}$$

To find the self-adjoint operator h from (5.3), we start with the quadratic form (5.44). Inserting (5.64) into the latter and performing several integrations by parts with noticing that $LM = -L - M$ and $(M\psi)' = -i\alpha M\psi - i\alpha\psi$ results in:

$$t_h[\psi] = \|\psi'\|^2 + \alpha^2 |\langle \chi_0^N, \psi \rangle|^2. \tag{5.65}$$

The corresponding operator h reads:

$$
\begin{aligned}
h\psi &= -\psi'' + \alpha^2 \chi_0^N \langle \chi_0^N, \psi \rangle, \\
\mathsf{D}(h) &= \left\{ \psi \in W^{2,2}(-a,a) : \psi'(\pm a) = 0 \right\}.
\end{aligned}
\tag{5.66}
$$

We remark that h is a rank one perturbation of the Neumann Laplacian. The eigenfunctions of h are χ_n^N with χ_0^N corresponding to the eigenvalue α^2.

It is interesting to compare the spectra of H and h for $\alpha = k_n$, *i.e.* in the points where the spectra are degenerate and similarity transformation breaks down because the operator Ω is not invertible. k_n^2 is an eigenvalue with the algebraic multiplicity two for both H and h. However, the geometric multiplicity differs: it is one for H and two for h.

The form of h also explains the origin of the peculiar α-dependence of the eigenvalues of H (which are all constant except for $\lambda_0(\alpha) = \alpha^2$). In fact, it is the nature of the rank one perturbation to leave all the Neumann eigenvalues untouched except for the lowest one that is driven to the α^2 behaviour.

5.4.5 More general boundary conditions

Finally, we consider the general $\mathcal{PT}$-symmetric boundary conditions $c_\pm := \mathrm{i}\alpha \pm \beta$, with $\alpha, \beta \in \mathbb{R}$. We start with formal considerations. The Θ-self-adjointness of H can be expressed in the following way. We take the advantage of the realization of $\Theta = I + K$, which we insert into $\Theta H \psi = H^* \Theta \psi$, $\psi \in \mathsf{D}(H)$. A formal interchange of differentiation with integration and integration by parts yield following problem that we can understand in distributional sense:

$$
(\partial_x^2 - \partial_y^2)\mathcal{K}(x,y) = 0, \tag{5.67}
$$

$$
\partial_y \mathcal{K}(x, \pm a) + (\mathrm{i}\alpha \pm \beta)\mathcal{K}(x, \pm a) = 0. \tag{5.68}
$$

Moreover, $\Theta\psi$ must belong to $\mathsf{D}(H^*)$, from which we have a condition

$$
\partial_x \mathcal{K}(\pm a, y) + (-\mathrm{i}\alpha \pm \beta)\mathcal{K}(\pm a, y) = 2\mathrm{i}\alpha\delta(y \mp a). \tag{5.69}
$$

Here δ denotes the Dirac delta function.

Already presented examples of Θ for $\beta = 0$ satisfy these requirements, particularly $\mathcal{K}$ solves the wave equation (5.67). The kernel (5.60), corresponding to the simpler form of presented metric operators, is a function of $x - y$ only. Inspired by this, we find the solution of the wave equation

$$
\mathcal{K}(x,y) = e^{\mathrm{i}\alpha(x-y) - \beta|x-y|} \left[c + \mathrm{i}\alpha \, \mathrm{sgn}(x-y) \right], \quad c \in \mathbb{R}, \tag{5.70}
$$

that satisfies the "boundary conditions" (5.68) and (5.69) as well. The one parametric family of solutions (5.70) of (5.67)–(5.69) demonstrates the known non-uniqueness of solutions to this problem. We also remark that c can be taken as α or a dependent as well.

The positivity of Θ is ensured if the norm of K is smaller than 1. This can be estimated by the Hilbert-Schmidt norm of K which is explicitly computable:

$$
\|K\|_{\mathrm{HS}}^2 = (c^2 + \alpha^2) \, \frac{4a\beta + e^{-4a\beta} - 1}{2\beta^2} \tag{5.71}
$$

(with the convention that if $\beta = 0$ one should take the limit of the right hand side as $\beta \to 0$). Consequently, the positivity of Θ can be achieved by several ways, *e.g.*, if a is small; or if β is positive and large; or $|c|$ and $|\alpha|$ are small. In any of the regimes, the formal manipulations above are justified.

Let us summarize the results of this subsection into the following theorem.

Theorem 5.3. *Let $c_\pm := \mathrm{i}\alpha \pm \beta$, with $\alpha, \beta \in \mathbb{R}$, and assume that all the eigenvalues of H are simple. Moreover, let $\|K\|_{\mathrm{HS}} < 1$, where K is a Hilbert-Schmidt operator with the explicit kernel* (5.70) *and $\|K\|_{\mathrm{HS}}$ is explicitly computed in* (5.71). *Then $\Theta := I + K$ is a metric operator for H.*

5.5 Bounded perturbations

In this section we show that results of Section 5.3 remain valid if we consider a bounded perturbation V of H.

Firstly we remark that the perturbation result [13, Thm. XIX 2.7] guarantees that $H + V$ remains a discrete spectral operator. That is, if all the eigenvalues of $H + V$ are simple, then the metric operator Θ exists. We show that the claim of Theorem 5.1 is valid for $H + V$ as well. The rest of the results from Section 5.3 then follows straightforwardly. The approach is to use analytic perturbation theory for the operator $h := \Omega H \Omega^{-1}$ that is perturbed by a bounded operator $\Omega V \Omega^{-1}$.

Theorem 5.4. *Let V be a bounded operator defined on the whole Hilbert space $\mathcal{H}$. Assume that all the eigenvalues of both the operators H and $H+V$ are simple. We denote by ξ_n, η_n the eigenfunctions of $H+V$ and H^*+V^*, respectively. Let e_n be elements of any orthonormal basis in $\mathcal{H}$. Then $\Omega_V = \sum_{n=0}^{\infty} e_n\langle\eta_n,\cdot\rangle$,* i.e. *$\Omega_V : \xi_n \mapsto e_n$, can be expressed as*

$$\Omega_V = U + L, \tag{5.72}$$

where U is a unitary operator and L is a Hilbert-Schmidt operator.

Proof. As in the proof of Theorem 5.1, without loss of generality, we restrict ourselves to $e_n := \chi_n^N$ and we show that $\Omega_V = I + L$ with L being Hilbert-Schmidt. We consider the normal operator $h := \Omega H \Omega^{-1}$ and we perturb it by $v := \Omega V \Omega^{-1}$. More specifically, we construct $h(\varepsilon) := h + \varepsilon\, v$ forming a holomorphic family of type (A) with respect to the parameter ε. We denote by $\mu_n(\varepsilon)$, $\overline{\mu_n(\varepsilon)}$ the eigenvalues and by $\tilde{\xi}_n(\varepsilon)$, $\tilde{\eta}_n(\varepsilon)$ the corresponding eigenfunctions of $h(\varepsilon)$ and of $h(\varepsilon)^*$ respectively. $h(0)$, $h(0)^*$ are normal, therefore the eigenfunctions $\tilde{\xi}_n(0)$ and $\tilde{\eta}_n(0)$ form orthonormal bases. In fact, with our choice of e_n, $\tilde{\xi}_n(0) = \tilde{\eta}_n(0) = \chi_n^N$.

We construct operator $\tilde{\Omega} : \tilde{\xi}_n(1) \mapsto \chi_n^N$ and we will show that $\tilde{\Omega} = I + \tilde{L}$, where $\tilde{L}$ is Hilbert-Schmidt. Ω_V is the composition of Ω and $\tilde{\Omega}$ and the claim then follows easily using of the fact that Hilbert-Schmidt operators are a *-both-sided ideal.

The distance of $\mu_n(0)$ and $\mu_n(1)$ can be at most $\|v\|$. Since we know the asymptotics of $\mu_n(0) = \lambda_n$, see (5.30), it is clear that there exists N_0 such that for all $n > N_0$, $|\mu_{n+1}(1) - \mu_n(1)| > n$ holds. Moreover, for such n the radius of convergence of perturbation series for eigenvalues and eigenfunctions is larger than 1. Thus, we have

$$\tilde{\eta}_n(\varepsilon) = \chi_n^N + \sum_{j=1}^{\infty} \tilde{\eta}_n^{(j)} \varepsilon^j. \tag{5.73}$$

We estimate the norms of $\tilde{\eta}_n^{(j)}$ using the analytic perturbation theory:

$$\begin{aligned} \|\tilde{\eta}_n^{(j)}\| &\leq \frac{1}{2\pi} \oint_{\Gamma_n} \left\| (h(0)^* - E)^{-1} (v^*(h(0)^* - E)^{-1})^j \chi_n^N \right\| \mathrm{d}E \\ &\leq \frac{1}{2\pi} \oint_{\Gamma_n} \frac{2^{j+1}\|v\|^j}{n^{j+1}} \mathrm{d}E \leq \frac{c^j}{n^j}, \end{aligned} \tag{5.74}$$

where Γ_n is a circle around $\mu_n(0)$ of radius $n/2$ and the constant c does not depend on n. We define N_1 as such that $N_1 \geq N_0$ and $c/N_1 < 1$.

We prove that $\tilde{\Omega}$ has the desired form by showing that the adjoint $\tilde{\Omega}^* = \sum_{n=0}^{\infty} \tilde{\eta}_n(1)\langle\chi_n^N,\cdot\rangle$ can be written as $\tilde{\Omega}^* = I + \tilde{L}_{N_1}^* + \tilde{L}_\infty^*$, where

$$\tilde{L}_{N_1}^* := \sum_{n=0}^{N_1-1} (\tilde{\eta}_n(1) - \chi_n^N)\langle\chi_n^N,\cdot\rangle, \quad \tilde{L}_\infty^* := \sum_{n=N_1}^{\infty} \sum_{j=1}^{\infty} \tilde{\eta}_n^{(j)} \langle\chi_n^N,\cdot\rangle, \tag{5.75}$$

and $\tilde{L}_{N_1}^*$ and $\tilde{L}_\infty^*$ are Hilbert-Schmidt. The decomposition of $\tilde{\Omega}^*$ follows immediately if we consider the expansions (5.73) for $n > N_1$ and rewrite $\tilde{\eta}_n(1) = \chi_n^N + (\tilde{\eta}_n(1) - \chi_n^N)$ for $n \leq N_1$. $\tilde{L}_{N_1}^*$ is a finite rank operator therefore it is obviously Hilbert-Schmidt. $\tilde{L}_\infty^*$ is bounded and the defining sum is absolutely convergent since

$$\begin{aligned} \sum_{n=N_1}^{\infty} \sum_{j=2}^{\infty} \|\tilde{\eta}_n^{(j)}\| |\langle\chi_n^N,\psi\rangle| &\leq \|\psi\| \sum_{n=N_1}^{\infty} \sum_{j=2}^{\infty} \left(\frac{c}{n}\right)^j \leq \|\psi\| \sum_{n=N_1}^{\infty} \frac{c^2}{n^2 - nc}, \\ \sum_{n=N_1}^{\infty} \|\tilde{\eta}_n^{(1)}\| |\langle\chi_n^N,\psi\rangle| &\leq c \sqrt{\sum_{n=N_1}^{\infty} \frac{1}{n^2}} \sqrt{\sum_{n=N_1}^{\infty} |\langle\chi_n^N,\psi\rangle|^2} \leq c\|\psi\| \sqrt{\sum_{n=N_1}^{\infty} \frac{1}{n^2}}. \end{aligned} \tag{5.76}$$

Finally we estimate the Hilbert-Schmidt norm of $\tilde{L}_\infty^*$:

$$\begin{aligned} &\sum_{p=0}^{\infty} \left\langle \sum_{m=N_1}^{\infty} \sum_{i=1}^{\infty} \tilde{\eta}_m^{(i)} \langle\chi_m^N,\chi_p^N\rangle, \sum_{n=N_1}^{\infty} \sum_{j=1}^{\infty} \tilde{\eta}_n^{(j)} \langle\chi_n^N,\chi_p^N\rangle \right\rangle \\ &\leq \sum_{p=N_1}^{\infty} \sum_{i=1}^{\infty} \left(\frac{c}{p}\right)^i \sum_{j=1}^{\infty} \left(\frac{c}{p}\right)^j \leq \sum_{p=N_1}^{\infty} \left(\frac{c}{p-c}\right)^2 < \infty. \end{aligned} \tag{5.77}$$

This concludes the proof of the theorem. □

Remark 5.6 (General Sturm-Liouville operators)**.** Let us conclude this section by a remark on how to extend the previous result on bounded perturbations V for the operator H in the general form

$$H\psi := -(\rho\psi')' + V\psi \qquad \text{on} \qquad L^2(-a,a)\,,$$

subject to the boundary conditions

$$\rho(\pm a)\psi'(\pm a) + c_\pm \psi(\pm a) = 0. \tag{5.78}$$

Assuming merely that ρ is a bounded and uniformly positive function, *i.e.*, there exists a positive constant C such that $C^{-1} \leq \rho(x) \leq C$ for all $x \in (-a,a)$, the operator can be defined (*cf* [10, Corol. 4.4.3]) as an m-sectorial operator associated with a closed sectorial form with domain $W^{1,2}(-a,a)$. If, in addition, we assume that $\rho \in W^{1,\infty}(-a,a)$, then it is possible to check that the domain of H consists of functions ψ from the Sobolev space $W^{2,2}(-a,a)$ satisfying (5.78).

Now, let us strengthen the regularity hypothesis to $\rho \in W^{2,\infty}(-a,a)$ and introduce the unitary (Liouville) transformation $\mathcal{U} : L^2(-a,a) \to L^2(f(-a), f(a))$ by

$$\mathcal{U}^{-1}\phi := \rho^{-1/4}\,\phi \circ f\,, \qquad \text{where} \qquad f(x) := \int_0^x \frac{d\xi}{\sqrt{\rho(\xi)}}\,.$$

Then it is straightforward to check that the unitarily equivalent operator $\tilde{H} := \mathcal{U}H\mathcal{U}^{-1}$ on $L^2(f(-a), f(a))$ satisfies

$$\begin{aligned}
\tilde{H}\phi &= -\phi'' + \tilde{V}\phi + W\phi,\\
\mathsf{D}(\tilde{H}) &= \big\{\phi \in W^{2,2}\big(f(-a), f(a)\big) :\ \phi'(\pm f(a)) + \tilde{c}_\pm \phi(\pm f(a)) = 0\big\},
\end{aligned}$$

where $\tilde{V} := \mathcal{U}V\mathcal{U}^{-1}$ and

$$\tilde{c}_\pm := \frac{c_\pm}{\rho(\pm a)^{1/4}} - \frac{1}{4}\frac{\rho'(\pm a)}{\rho(\pm a)^{1/2}}\,, \qquad W := \left(\frac{1}{4}\rho'' - \frac{1}{16}\frac{\rho'^2}{\rho}\right) \circ f^{-1}\,.$$

In this way, we have transformed the second-order perturbation represented by ρ into a bounded potential W and modified boundary conditions. Theorem 5.4 applies to $\tilde{H}$ and, as a consequence of the unitary transform $\mathcal{U}$, to H as well.

5.6 Conclusions

In this article, we investigated properties of the similarity transformations Ω and metric operators Θ for Sturm-Liouville operators with separated, Robin-type boundary conditions, and the structure of the normal or self-adjoint operators to which they are similar.

We would like to mention that Θ and Ω cannot be always expressed as the sum of the identity and a Hilbert-Schmidt operator for other types of (differential) operators, see, *e.g.*, [2, 43, 33, 18], where Θ is a sum of the identity and a bounded non-compact operator. The latter is a composition of the parity and the multiplication by sign function. Moreover, corresponding similarity transformations map (non-self-adjoint) point interactions to (self-adjoint) point interactions, which is not typically the case for operators studied here. This is illustrated in the example of $\mathcal{PT}$-symmetric boundary conditions where the equivalent self-adjoint operator is not a point interaction but rather a rank one perturbation of the Neumann Laplacian.

In this work we considered the separated boundary conditions only. Nonetheless, the analogous results are expected to be valid for all strongly regular boundary conditions.

The crucial property is the asymptotics of eigenvalues, *i.e.* separation distance of eigenvalues tends to infinity, that is used for the proof of the existence of similarity transformations [13]. Recent results on basis properties for perturbations of harmonic oscillator type operators [1, 41, 3] give a possibility to investigate the structure of similarity transformation in these cases as well. Another step is to consider *e.g.* on Hill operators, where a criterion on being spectral operator of scalar type has been obtained in [16] and recently extended in [12]. On the other hand, the structure of similarity transformations for operators with continuous spectrum as well as for multidimensional Schrödinger operators is almost unexplored and constitutes thus a challenging open problem.

In case of the $\mathcal{PT}$-symmetric boundary conditions, we found all the studied objects in a closed formula form, which is hardly the case in more general situations. However, in general, we may search for approximations of Ω or Θ, typically applying the analytic perturbation theory to find perturbation series for eigenvalues and eigenfunctions of H to certain order k. For instance, we perturb the parameters $c_\pm$ in boundary conditions by small ε. As a result we find an approximation h_{app} of the similar operator h with resolvents satisfying $\|(h-z)^{-1} - (h_{\text{app}} - z)^{-1}\| \leq C\varepsilon^k$. An extensive discussion and example of such construction can be found in [46]. The same remark is appropriate for small perturbations by bounded operator discussed in Section 5.5.

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Chapter 6

Perfect transmission scattering as a $\mathcal{PT}$-symmetric spectral problem

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Perfect transmission scattering as a $\mathcal{PT}$-symmetric spectral problem

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Abstract. We establish that a perfect-transmission scattering problem can be described by a class of parity and time reversal symmetric operators and hereby we provide a scenario for understanding and implementing the corresponding quasi-Hermitian quantum mechanical framework from the physical viewpoint. One of the most interesting features of the analysis is that the complex eigenvalues of the underlying non-Hermitian problem, associated with a reflectionless scattering system, lead to the loss of perfect-transmission energies as the parameters characterizing the scattering potential are varied. On the other hand, the scattering data can serve to describe the spectrum of a large class of Schrödinger operators with complex Robin boundary conditions.

6.1 Introduction

Recently there has been a considerable amount of work devoted to the study of the so-called $\mathcal{PT}$-symmetric quantum mechanics – see [1, 13] and the references therein. The theory is based on the idea to give a physical meaning to a class of non-Hermitian Hamiltonians being symmetric under the composed space reversal transformation $\mathcal{P}$ and complex conjugation $\mathcal{T}$. These Hamiltonians are interesting because some of them have exclusively real spectrum and – usually only after an appropriate change of the inner product of Hilbert space – they can generate unitary time-evolution. The relevance of $\mathcal{PT}$-symmetric operators has been suggested in various domains of physics: nuclear physics [18], optics [6, 11, 19, 20], solid state [2], superconductivity [14, 15], and electromagnetism [16, 12]. Moreover, the first experimental results in optics using the formalism of $\mathcal{PT}$-symmetric quantum mechanics in the theoretical explanation of observed effects have appeared recently [10, 4, 17].

In this letter, we establish a purely quantum-mechanical interpretation of a class of $\mathcal{PT}$-symmetric Hamiltonians in a particular scattering problem. Hereby we confirm the common claim that the non-Hermiticity corresponds to gain/loss mechanisms of probability density and that the presence $\mathcal{PT}$-symmetry ensures the balance between these opposite effects [20, 2]. We show that the spectral techniques for non-self-adjoint (NSA) problems can be used for describing a scattering system in the reflectionless regime.

The general idea is that the above kind of scattering problems can be described by an effective Schrödinger equation in a bounded interval (corresponding to the domain of the scatterer) subject to complex Robin boundary conditions. This problem can be regarded as a particular class of $\mathcal{PT}$-symmetric quantum problems if the scattering potential respects such a symmetry. The gain/loss mechanism referred to above is clearly understood in this case, since we start with a Hermitian physical system and we can keep track of where and how the probability is lost or gained. Furthermore, the typical complex points appearing in the spectra of the NSA problems have a very natural explanation: they give rise to the loss of the perfect-transmission energies (PTEs). Finally, we solve the inverse problem, *i.e.* how the spectrum of a $\mathcal{PT}$-symmetric problem can be determined from the knowledge of PTEs.

We will conclude with the statement that the real points in the spectra of certain class of $\mathcal{PT}$-symmetric Hamiltonians can be *measured* in the quantum mechanical scattering problem and the points where two eigenvalues coalesce (exceptional points) correspond to the loss of PTEs.

6.2 From scattering to spectral theory

Consider a quantum particle of mass m scattered by a potential of the form $V(x, y, z) = v(x)$, for a general real-valued function v supported in $[-a, a]$ with $a > 0$. We shall restrict ourselves to scattering waves in the x-direction, so that the problem can be described by the one-dimensional Schrödinger equation

$$-\psi''(x) + v(v)\psi(x) = k^2\psi(x), \tag{6.1}$$

where ψ is the particle wavefunction and k a positive (wave)number. Since v is zero outside $[-a, a]$, we have the asymptotic solutions: $\psi_l(x) = \exp(ikx) + R\exp(-ikx)$ for the in-coming wave (for $x \le -a$), and $\psi_r(x) = T\exp(ikx)$ for the out-coming wave (for $x \ge a$), where R and T correspond to the reflection and transmission amplitudes, respectively. Note that we consider only the special solutions for which the incident amplitude is equal to one.

Now we explain how the state ψ of the particle can be described by an effective Schrödinger equation in the interval $[-a, a]$. We focus on the special case of perfect-transmission, *i.e.* $R = 0$. By plugging $R = 0$ in the in-coming wave and requiring the continuity of ψ and its derivative at the boundary $\pm a$, it is easy to show that the scattering problem is then equivalent to the non-linear (energy dependent) problem (in units where $m = 1/2$ and $\hbar = 1$)

$$\begin{aligned} -\psi''(x) + v(x)\psi(x) &= k^2\psi(x), \qquad \forall x \in [-a, a], &(6.2)\\ \psi'(\pm a) - ik\psi(\pm a) &= 0. &(6.3)\end{aligned}$$

The non-linear problem (6.2)–(6.3) can be solved by considering the associated one-parametric (linear) spectral problem:

$$\begin{aligned} -\psi''(x) + v(x)\psi(x) &= \mu(\alpha)\psi(x), \quad \forall x \in [-a, a], &(6.4)\\ \psi'(\pm a) - i\alpha\psi(\pm a) &= 0. &(6.5)\end{aligned}$$

In the above expression, $\mu(\alpha)$ plays the role of eigenvalue and α is a real parameter. The energies corresponding to the perfect-transmission states are found as those points $\mu(\alpha_*)$ satisfying

$$\mu(\alpha_*) = \alpha_*^2. \tag{6.6}$$

The relation (6.5) is the so-called $\mathcal{PT}$-symmetric Robin boundary condition and it has been studied before in the context of spectral theory for NSA operators [8, 7, 9]. These boundary conditions have been used previously in the phenomenological description of emission and absorption, however, here they appear naturally in the scattering and in the framework of spectral theory for $\mathcal{PT}$-symmetric (or more general NSA) operators. Moreover, since the boundary conditions (6.5) imply that the probability current at $x = \pm a$ does not vanish (for $\alpha \neq 0$), the non-self-adjointness in this system can be clearly understood as the gain/loss of probability density at the boundary points. Furthermore, the $\mathcal{PT}$ symmetry is a consequence of our restriction to the reflectionless regime, which corresponds to the exact compensation of the gains and losses.

6.3 Square well potential

We illustrate our approach on the explicitly solvable model of the square well

$$v(x) = -v_0\chi_{[-a,a]}(x), \tag{6.7}$$

where $\chi_A(x)$ is the characteristic (or indicator) function of a set A and $v_0 > 0$. The eigenvalues of the corresponding NSA problem (6.4)–(6.5) with the above potential are given by (see [8]):

$$\mu_n = \begin{cases} \alpha^2 - v_0, & n = 0, \\ (\frac{n\pi}{2a})^2 - v_0, & n \in \mathbb{N}. \end{cases} \tag{6.8}$$

Therefore, by employing the knowledge of the spectrum of the Hamiltonian and taking into account expression (6.6), we get indeed the well-known PTEs for the square well potential $k^2 = (\frac{n\pi}{2a})^2 - v_0$ (see *e.g.*, [3]).

The first three PTEs, corresponding to the intersection of the graphics $\mu_n(\alpha)$ and expression (6.6), are presented in Figure 6.1. If the potential depth v_0 tends to zero, the continuous (red) parabola corresponding to the eigenvalue μ_0 approaches the dashed (blue) parabola representing dispersion relation (6.6). The two parabolas coincide when $v_0 = 0$, *i.e.* with no potential all positive energies trivially correspond to perfect transmission.

6.4 Multiple steps potential

We claim that the presence of complex eigenvalues lead to observable effects. We demonstrate this on models with even piecewise constant potentials

$$v(x) = \sum_{j=1}^{N+1} \beta_j \varepsilon_j^{-1} \chi_{[x_{j-1}, x_j]}(|x|), \tag{6.9}$$

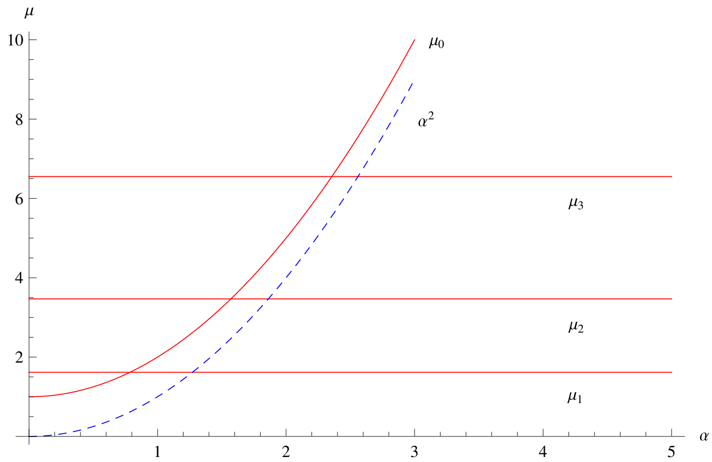

Figure 6.1: The spectrum of the square well potential with $v_0 = -1$ and $a = 2$. The dashed (blue) curve represents the dispersion relation curve $\mu = \alpha^2$ while the continuous (red) lines are the energy levels. The PTEs correspond to the intersections of the constant μ_n's with the dispersion parabola.

where $0 \leq x_0 < \cdots < x_N \leq a$, $\varepsilon_j = x_j - x_{j-1}$ determine the width and β_j the strength of the constant parts. This type of solvable models – as usual by using the explicitly known wavefunctions in the intervals where the potential is constant and matching them at the interface points – can serve as approximation to realistic physical potentials which also fit to our framework.

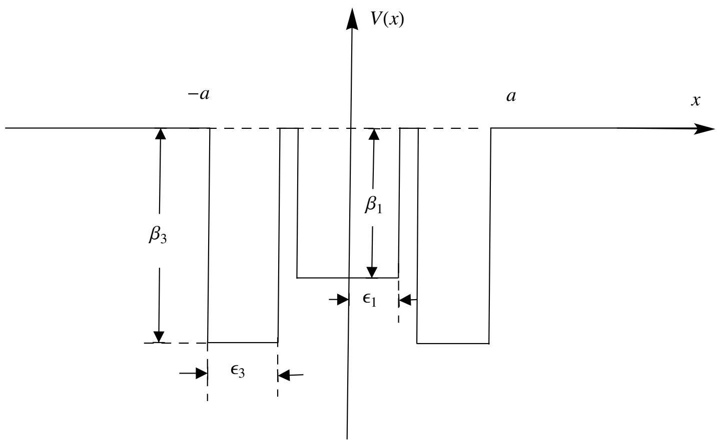

Figure 6.2: The shape of considered multiple steps potential.

We focus on $N = 2$ model with $x_0 = 0, x_3 = a$ and $\beta_1 < 0$, $\beta_2 = 0$, $\beta_3 \neq 0$, *i.e.* two steps localized at the endpoints and one at the origin, see Figure 6.2, however, our reasoning is not limited to this particular solvable potential. Inspired by the delta-interaction models [9] that are limits of the considered potentials for a special choice of parameters, it is not surprising that complex conjugated pairs of eigenvalues are present in the spectrum. Intersections of the dispersion parabola (6.6) and energy levels represent PTEs, *cf.* Figure 6.3. However, there is no PTE corresponding to the intersection with complex energy since $\mu = k^2$ is required to be real (to have in-coming and out-coming plane waves e^{ikx}).

The shape of the energy curves $\mu_n(\alpha)$ depends on the potential and we prepare such scenario (by fixing the steps at the endpoints and changing the strength of the one in the middle) that the dispersion parabola intersects at first two energy levels, then precisely the point of complexification (or exceptional point), and finally the complex level. Figure 6.4 illustrates the resulting behavior of PTEs, two originally separated PTEs merge when the intersection is the complexification point and then completely disappear, see animation [5].

This process can be also described in terms of the transmission coefficient. The comparison of the two curves in Figure 6.5 (corresponding to different values of β_1) indicate how the process can be observed from scattering data: two initially separated peaks (PTEs), *e.g.* around $k^2 \approx 160$ in the continuous red line, collide as β_1 is varied (complexification point is intersected by the dispersion parabola) and fall down afterwards (a loss of PTEs) around $k^2 \approx 180$ in the dashed blue line. Broad peaks close to $|T|^2 = 1$, *e.g.* around $k^2 = 460$, correspond to the collision of PTEs (approaching the complexification point).

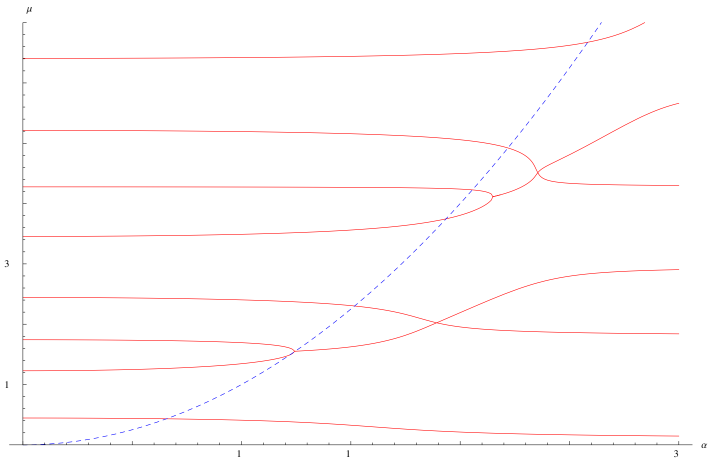

Figure 6.3: The real part of the eigenvalue μ as a function of the parameter α for the step-like potential v with $a = \pi/4$, $\varepsilon_1 = 0.2$, $\varepsilon_3 = 0.5$, $\beta_1 = -90$, $\beta_2 = 0$, $\beta_3 = -100$. The PTEs correspond to the intersections of the energy levels (continuous, red) and the dispersion relation (dashed, blue).

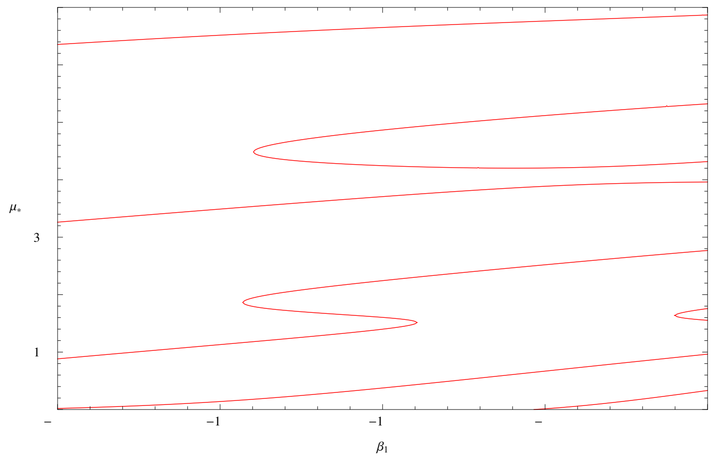

Figure 6.4: The PTEs μ_* as a function of β_1 for the step-like potential v with $a = \pi/4$, $\varepsilon_1 = 0.2$, $\varepsilon_3 = 0.5$, $\beta_3 = -100$, and $\beta_2 = 0$. The losses of PTEs are clearly visible *e.g.* around $\beta_1 = -140$, for $\mu_* \approx 190$ and $\mu_* \approx 450$.

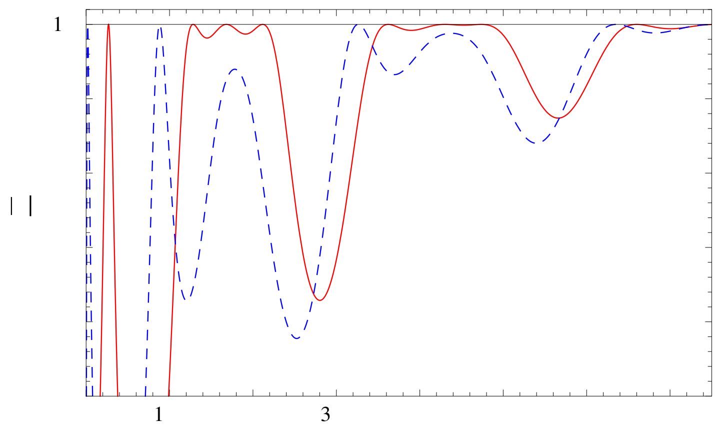

Figure 6.5: Transmissions $|T|^2$ as a function of energy k^2 for the step-like potential v with $a = \pi/4$, $\varepsilon_1 = 0.2$, $\varepsilon_3 = 0.5$, $\beta_3 = -100$, $\beta_2 = 0$, $\beta_1 = -120$ (continuous red line), and $\beta_1 = -200$ (dashed blue line). See [5] for animated plots of $|T|^2$ as a function of potential.

6.5 Inverse problem

Now let us explore the inverse problem, *i.e.* how we can determine the spectrum of a given $\mathcal{PT}$-symmetric (or more general NSA) Hamiltonian subject to complex Robin boundary conditions by measuring the PTEs in a scattering experiment. Consider the NSA problem defined by expressions (6.4)–(6.5) together with the dispersion relation (6.6) and let us modify it by adding a constant v_0 to the potential, *i.e.* putting the system into a square well, as follows:

$$-\psi''(x) + (v(x) + v_0)\psi(x) = \mu_0(\alpha)\psi(x), \tag{6.10}$$
$$\psi'(\pm a) - i\alpha\psi(\pm a) = 0, \tag{6.11}$$
$$\mu_0(\alpha) = \alpha^2. \tag{6.12}$$

The above problem can be recast as

$$-\psi''(x) + v(x)\psi(x) = \mu(\alpha)\psi(x), \tag{6.13}$$
$$\psi'(\pm a) - i\alpha\psi(\pm a) = 0, \tag{6.14}$$
$$\mu(\alpha) = \alpha^2 - v_0, \tag{6.15}$$

where we have introduced $\mu(\alpha) := \mu_0(\alpha) - v_0$. Clearly, (6.13)–(6.14) is *the same spectral problem* as the initial one (6.4)–(6.5), however, by comparing expressions (6.6) and (6.15), we see that the dispersion parabola is shifted by v_0.

Now, consider measurements of the PTEs corresponding to the choice of v_0, which we assume to be discrete for every v_0. Let us choose a PTE and denote by $\kappa(v_0)$ its v_0-dependence. Thus we have a function $v_0 \mapsto \kappa(v_0)$. It is clear from (6.10)–(6.15) that $\kappa(v_0) - v_0$ is the eigenvalue for the spectral problem (6.13)–(6.14) with α satisfying $\alpha^2 = \kappa(v_0)$. Hence we can obtain the entire α-dependence of the chosen energy level $\mu(\alpha)$ if κ is an invertible function. Indeed, for every α, we find $v_0 = \kappa^{-1}(\alpha^2)$ such that $\mu(\alpha) = \alpha^2 - \kappa^{-1}(\alpha^2)$ is the eigenvalue of (6.13)–(6.14).

It remains to ensure that κ is invertible, which follows if $\kappa'(v_0) \neq 0$ for all v_0. For all v_0, we have $\kappa(v_0) = \mu(\alpha) + v_0$, with $\alpha^2 = v_0$. By differentiating this relation with respect to v_0, we obtain $\kappa'(v_0) = 2\alpha/(2\alpha - \mu'(\alpha))$. The situation $2\alpha = \mu'(\alpha)$ is very particular: $\mu(\alpha)$ is (at least) locally parabola, thus it represents either reflectionless setting (the dispersion parabola (6.15) locally coincides with the energy level $\mu(\alpha)$) or no perfect transmission (no intersection of the energy level $\mu(\alpha)$ and (6.15)). Besides these exceptional cases we have obtained the condition on the spectrum of (6.13)–(6.14) $|\mu'(\alpha)| < \infty$ that assures invertibility of κ. This condition is however satisfied for all real α, except possibly for the points where energy levels cross, because of the analyticity of $\mu(\alpha)$, which is ensured for all relatively form bounded potentials v.

This means that we can determine the spectrum of the problem (6.13)–(6.14) by *measuring* the PTEs as a function of v_0. Of course, by this procedure we can only determine the real eigenvalues of the corresponding spectrum. The appearance of a complex conjugate pair of eigenvalues can be traced back as a loss of two (close) PTEs, analogously for the restoration of two real eigenvalues.

6.6 Discussion and conclusions

We have shown that NSA Hamiltonians naturally arise in the effective description of a class of scattering problems. Within this context, we have proposed a spectral-type scheme for obtaining the energies corresponding to a perfect-transmission scattering process. The model confirms the common claim that $\mathcal{PT}$-symmetric operators describe physical systems where the probability density is not conserved locally, but the gains and losses compensate globally. The appearance of complex eigenvalues in the associated $\mathcal{PT}$-symmetric spectral problem – resulting from the collision of a pair of real ones – can lead to the merging and subsequent disappearance of two PTEs which, moreover, can be observed in a scattering experiment. Furthermore, we have discussed the inverse problem, that is, how to use the scattering data to determine the spectrum of an operator with non-Hermitian boundary conditions.

It is important to stress that the general idea of reducing a scattering problem to a non-linear eigenvalue equation is not limited to even potentials (ensuring the $\mathcal{PT}$-symmetry) and the $\mathcal{PT}$-symmetric Robin-type boundary conditions (reflecting the perfect-transmission process). However, when $\mathcal{PT}$-symmetry is relaxed, real energy levels do not need to cross anymore to produce complex eigenvalues and therefore the overall analysis of the spectrum of the associated NSA operator is more complicated.

The main purpose of this letter was to establish a truly quantum-mechanical interpretation of a $\mathcal{PT}$-symmetric model. Furthermore, we believe that the associated spectral framework of perfect-transmission process provides an additional insight to effects that can be observed in scattering data.

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Chapter 7

$\mathcal{PT}$-symmetric models in curved manifolds

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$\mathcal{PT}$-symmetric models in curved manifolds

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Abstract. We consider the Laplace-Beltrami operator in tubular neighbourhoods of curves on two-dimensional Riemannian manifolds, subject to non-Hermitian parity and time preserving boundary conditions. We are interested in the interplay between the geometry and spectrum. After introducing a suitable Hilbert space framework in the general situation, which enables us to realize the Laplace-Beltrami operator as an m-sectorial operator, we focus on solvable models defined on manifolds of constant curvature. In some situations, notably for non-Hermitian Robin-type boundary conditions, we are able to prove either the reality of the spectrum or the existence of complex conjugate pairs of eigenvalues, and establish similarity of the non-Hermitian m-sectorial operators to normal or self-adjoint operators. The study is illustrated by numerical computations.

Mathematics Subject Classification (2010): 81Q12, 81Q35, 58J50, 34L40, 35P10

Keywords: Laplace-Beltrami operator, non-self-adjoint boundary conditions, Robin-type boundary conditions, real spectrum, Riesz basis, two-dimensional manifolds of constant curvature, J-self-adjointness, PT-symmetry

7.1 Introduction

Many systems in Nature can be under first approximation described by linear second order differential equations, such as the wave, heat or Schrödinger equation. The common denominator of them is the Helmholtz equation describing the stationary regime and leading to the spectral study of the Laplace operator. Already from the mathematical point of view, it is important to understand the influence of the geometry to the spectrum of the Laplacian, subject to various types of boundary conditions, and vice versa, to characterize geometric and boundary interface properties from given spectral data.

In this paper, we are interested in the interplay between the curvature of the ambient space and the spectrum of the Laplacian subjected to a special class of non-Hermitian boundary conditions. We choose probably the simplest non-trivial model, *i.e.*, the spectral problem corresponding to the equation

$$-\Delta\psi = \lambda\psi \qquad \text{in} \qquad \Omega\,, \tag{7.1}$$

where λ is a spectral parameter, Ω is an a-tubular neighbourhood of a closed curve Γ (usually a geodesic) in a two-dimensional Riemannian manifold $\mathcal{A}$ (not necessarily embedded in $\mathbb{R}^3$), *i.e.*,

$$\Omega := \{x \in \mathcal{A} \mid \operatorname{dist}(x,\Gamma) < a\}\,, \tag{7.2}$$

and $-\Delta$ is the associated Laplace-Beltrami operator. The boundary conditions we consider are general 'parity and time preserving' boundary conditions introduced in Section 7.2.3 below; a special example is given by the non-Hermitian Robin-type boundary conditions

$$\frac{\partial\psi}{\partial n} + i\alpha\psi = 0 \qquad \text{on} \qquad \partial\Omega\,, \tag{7.3}$$

where n is the curve normal translated by geodesics orthogonal to Γ and α is a real-valued function.

The Schrödinger equation in tubular neighbourhoods of submanifolds of curved Riemannian manifolds has been extensively studied in the context of quantum waveguides and molecular dynamics (*cf* [57] for a recent mathematical paper with many references). Here the confinement to a vicinity of the submanifold is usually modelled by constraining potentials [41, 57] or Dirichlet boundary conditions [14, 34, 35].

Note that, on the contrary, the non-Hermitian nature of boundary conditions (7.3) enables one to model a leak/supply of energy from/into the subsystem Ω, since the probability current does not vanishes on the boundary $\partial\Omega$ unless $\alpha = 0$. In fact, non-Hermitian boundary conditions of the type (7.3) has been considered in [31, 30, 29] to model open (dissipative) quantum systems. One also arrives at (7.3) when transforming a scattering problem to a (non-linear) spectral one [17, Ex. 9.2.4]. Quite recently it has been observed in [51] that the boundary conditions (7.3) appear in a supersymmetric counterpart of the one-dimensional quantum well. Finally, let us observe that Robin boundary conditions are known under the term impedance boundary conditions in classical electromagnetism, where they are conventionally used to approximate very thin layers [11, 19, 6].

Our primary motivation to consider the spectral problem (7.1), (7.3) comes from the so-called '$\mathcal{PT}$-symmetric quantum mechanics' originated by the paper [8], where the authors discussed a class of Schrödinger operators H in $L^2(\mathbb{R})$ whose spectrum is real in spite of the fact that their potentials are complex. They argued that the rather surprising reality of the spectrum follows from the $\mathcal{PT}$-symmetry property:

$$[H, \mathcal{PT}] = 0 . \tag{7.4}$$

Here the 'parity' $\mathcal{P}$ and 'time reversal' $\mathcal{T}$ operators are defined by $(\mathcal{P}\psi)(x) := \psi(-x)$ and $\mathcal{T}\psi := \overline{\psi}$. It is important to emphasize that $\mathcal{T}$ is an antilinear operator and that (7.4) is neither sufficient nor necessary condition to ensure the reality of the spectrum of H.

Nevertheless, later on it was observed in [9, 42, 43, 44] that if the spectrum of a $\mathcal{PT}$-symmetric operator H in a Hilbert space $\mathcal{H}$ is indeed real (and some further hypotheses are satisfied) the condition (7.4) actually implies that H is 'quasi-Hermitian' [52], *i.e.*, there exists a bounded invertible positive operator Θ with bounded inverse, called 'metric', such that

$$H^* = \Theta^{-1} H \Theta . \tag{7.5}$$

In other words, H is similar to a self-adjoint operator for which a conventional quantum-mechanical interpretation makes sense. We refer to recent reviews [7, 45] and proceedings [28, 5, 21] for further information and references about the concept of $\mathcal{PT}$-symmetry.

In addition to the potential quantum-mechanical interpretation, we would like to mention the relevance of $\mathcal{PT}$-symmetric operators in view of their recent study in the context of superconductivity [48, 49], electromagnetism [50, 33] and fluid dynamics [13, 16, 58, 12].

A suitable mathematical framework to analyse $\mathcal{PT}$-symmetric Hamiltonians is either the theory of self-adjoint operators in Krein spaces [39, 27] or the J-self-adjointness [10]. The latter means that there exists an antilinear involution J such that

$$H^* = JHJ . \tag{7.6}$$

The concept (7.6) is not restricted to functional Hilbert spaces and it turns out that the majority of $\mathcal{PT}$-symmetric Hamiltonians existing in the literature are indeed J-self-adjoint. In general, however, the properties (7.4), (7.5) and (7.6) are all unrelated [53, 55].

Summing up, given a non-Hermitian operator H satisfying (7.4), two fundamental questions arises. First,

1. is the spectrum of H real?

Second, if the answer to the previous question is positive,

2. does there exist a metric Θ satisfying (7.5)?

It turns out that the questions constitute a difficult problem in the theory of non-self-adjoint operators.

For this reason, one of the present authors and his coauthors proposed in [37] (see also [36]) an elementary one-dimensional $\mathcal{PT}$-symmetric Hamiltonian, for which the spectrum and metric are explicitly computable. The simplicity of the Hamiltonian consists in the fact that it acts as the Hamiltonian of a free particle in a box and the non-Hermitian interaction is introduced via the Robin-type boundary conditions (7.3) only. The model was later generalized to a two-dimensional waveguide in [10], where the variable coupling in the boundary conditions is responsible for existence of real (or complex conjugate pairs of) eigenvalues outside the essential spectrum (see also [38]).

In this paper we continue the generalization of the models of [37, 10] to curved Riemannian manifolds. This leads to a new, large class of $\mathcal{PT}$-symmetric Hamiltonians. Our main goal is to study the effect of curvature on the spectrum, namely the existence/absence of non-real eigenvalues and the metric.

The organization of this paper is as follows.

In the following Section 7.2, we introduce our model in a full generality, in the sense that the ambient geometry and boundary interaction of the spectral problem (7.1) are described by quite arbitrary (non-constant and non-symmetric) functions. Our main strategy to deal with the curved geometry is based on the usage of Fermi coordinates.

In Section 7.3, we use the framework of sesquilinear forms to define the Laplace-Beltrami operator appearing in (7.1) as a (closed) m-sectorial operator in the Hilbert space $L^2(\Omega)$. We also explicitly determine the operator domain if the assumptions about the geometry and boundary-coupling functions are naturally strengthen.

Moreover, we find conditions about the geometry under which the operator becomes $\mathcal{PT}$-symmetric (and $\mathcal{T}$-self-adjoint).

In order to study the effects of curvature on the spectrum, in Section 7.4 we focus on solvable models. Assuming that the curvature and boundary-coupling functions are constant, the eigenvalue problem can be reduced to the investigation of (infinitely many) one-dimensional differential operators with $\mathcal{PT}$-symmetric boundary conditions. Here the previous results [37, 36] and the general theory of boundary conditions for differential operators [46, 47] are appropriate and helpful. In particular, since the $\mathcal{PT}$-symmetric boundary conditions are (except one case excluded here by assumption) strongly regular ones, it is possible to show that the studied one-dimensional operators are 'generically' similar to self-adjoint or normal operators. However, it remains to decide whether this is true for their infinite sum, *i.e.*, for the original two-dimensional Laplace-Beltrami operator. To answer this in affirmatively, it turns out that the J-self-adjoint formulation of $\mathcal{PT}$-symmetry (*cf* the text around (7.6)) is fundamental, with $J = \mathcal{T}$ playing the role of antilinear involution. The properties of the solvable models are illustrated by a numerical analysis of their spectra.

The paper is concluded by Section 7.5 where possible directions of the future research are mentioned.

7.2 Definition of the model

We use the quantum-mechanical framework to describe our model.

7.2.1 The configuration space

We assume that the ambient space of a quantum particle is a connected complete two-dimensional Riemannian manifold $\mathcal{A}$ of class C^2 (not necessarily embedded in the Euclidean space $\mathbb{R}^3$). Furthermore, we suppose that the Gauss curvature K of $\mathcal{A}$ is continuous, which holds under the additional assumption that $\mathcal{A}$ is either of class C^3 or it is embedded in $\mathbb{R}^3$.

On the manifold, we consider a C^2-smooth unit-speed embedded curve $\Gamma : [-l, l] \to \mathcal{A}$, with $l > 0$. Since Γ is parameterized by arc length, the derivative $T := \dot{\Gamma}$ is the unit tangent vector of Γ. Let N be the unit normal vector of Γ which is uniquely determined as the C^1-smooth mapping from $[-l, l]$ to the tangent bundle of $\mathcal{A}$ by requiring that $N(s)$ is orthogonal to $T(s)$ and that $\{T(s), N(s)\}$ is positively oriented for all $s \in [-l, l]$ (*cf* [56, Sec. 7.B]). We denote by κ the corresponding curvature of Γ defined by the Frenet formula $\nabla_T T = \kappa N$, where ∇ stands for the covariant derivative in $\mathcal{A}$. We note that the sign of κ is uniquely determined up to the re-parametrization $s \mapsto -s$ of the curve Γ and that κ coincides with the geodesic curvature of Γ if $\mathcal{A}$ is embedded in $\mathbb{R}^3$.

The feature of our model is that the particle is assumed to be 'confined' to an a-tubular neighbourhood Ω of Γ, with $a > 0$. Ω can be visualized as the set of points q in $\mathcal{A}$ for which there exists a geodesic of length less than a from q meeting Γ orthogonally. More precisely, we introduce a mapping $\mathcal{L}$ from the rectangle

$$\Omega_0 := (-l, l) \times (-a, a) \equiv J_1 \times J_2 \tag{7.7}$$

(considered as a subset of the tangent bundle of $\mathcal{A}$) to the manifold $\mathcal{A}$ by setting

$$\mathcal{L}(x_1, x_2) := \exp_{\Gamma(x_1)}(N(x_1)\, x_2)\,, \tag{7.8}$$

where $\exp_q$ is the exponential map of $\mathcal{A}$ at $q \in \mathcal{A}$, and define

$$\Omega := \mathcal{L}(\Omega_0)\,. \tag{7.9}$$

Note that $x_1 \mapsto \mathcal{L}(x_1, x_2)$ traces the curves parallel to Γ at a fixed distance $|x_2|$, while the curve $x_2 \mapsto \mathcal{L}(x_1, x_2)$ is a geodesic orthogonal to Γ for any fixed x_1. See Figure 7.1.

7.2.2 The Fermi coordinates

Throughout the paper we make the hypothesis that

$$\boxed{\mathcal{L} : \Omega_0 \to \Omega \text{ is a diffeomorphism.}} \tag{7.10}$$

Since Γ is compact, (7.10) can always be achieved for sufficiently small a (*cf* [24, Sec. 3.1]). Consequently, $\mathcal{L}$ induces a Riemannian metric G on Ω_0, and we can identify the tubular neighbourhood $\Omega \subset \mathcal{A}$ with the Riemannian manifold (Ω_0, G). In other words, Ω can be conveniently parameterized via the (Fermi or geodesic parallel) "coordinates" (x_1, x_2) determined by (7.8). We refer to [24, Sec. 2] and [25] for the notion and

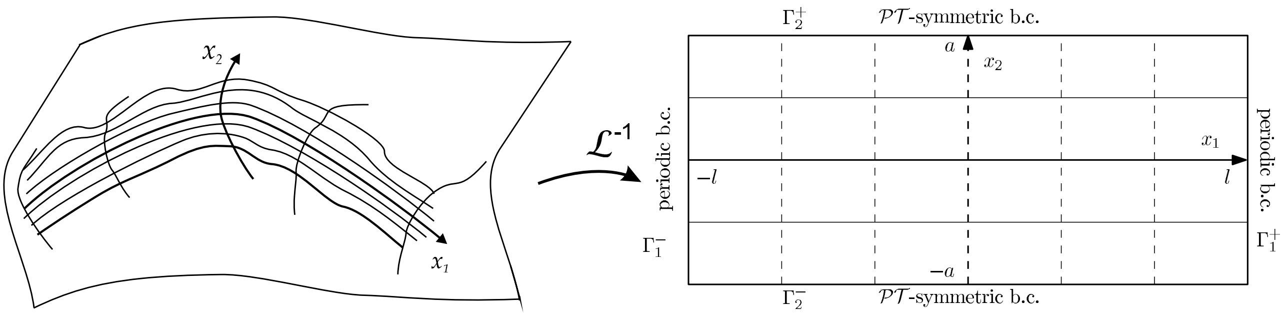


Figure 7.1: Strip and boundary conditions

properties of Fermi coordinates. In particular, it follows by the generalized Gauss lemma that the metric acquires the diagonal form:

$$G = \begin{pmatrix} f^2 & 0 \\ 0 & 1 \end{pmatrix}, \tag{7.11}$$

where f is continuous and has continuous partial derivatives $\partial_2 f$, $\partial_2^2 f$ satisfying the Jacobi equation

$$\partial_2^2 f + Kf = 0 \qquad \text{with} \qquad \begin{cases} f(\cdot,0) = 1\,, \\ \partial_2 f(\cdot,0) = -\,\kappa\,. \end{cases} \tag{7.12}$$

Here K is considered as a function of the Fermi coordinates (x_1, x_2).

7.2.3 The Hamiltonian

We identify the Hamiltonian H of the quantum particle in Ω with the Laplace-Beltrami operator $-\Delta_G$ in the Riemannian manifold (Ω_0, G), subject to a special class of non-self-adjoint boundary conditions.

The action of the Hamiltonian

Denoting by G^{ij} the coefficients of the inverse metric G^{-1} and $|G| := \det(G)$, we have

$$-\Delta_G = -|G|^{-1/2}\partial_i |G|^{1/2} G^{ij} \partial_j = -f^{-1}\partial_1 f^{-1}\partial_1 - f^{-1}\partial_2 f \partial_2\,. \tag{7.13}$$

Here the first equality (in which the Einstein summation convention is assumed) is a general formula for the Laplace-Beltrami operator $-\Delta_G$ expressed in local coordinates in a Riemannian manifold equipped with a metric G. The second equality uses the special form (7.11), for which $|G| = f^2$ and $G^{-1} = \operatorname{diag}(f^{-2}, 1)$. Henceforth we assume that the Jacobian of (7.10) is uniformly positive and bounded, *i.e.*,

$$\boxed{f, f^{-1} \in L^\infty(\Omega_0)\,,} \tag{7.14}$$

so that $-\Delta_G$ is a uniformly elliptic operator. Again, (7.14) can be achieved for sufficiently small a, *cf* (7.12).

Remark 7.1. The assumption (7.10) is not really essential. Indeed, abandoning the geometrical interpretation of Ω as a tubular neighbourhood embedded in $\mathcal{A}$, (Ω_0, G) with (7.11) can be considered as an abstract Riemannian manifold for which (7.14) is the only important hypothesis. The results of this paper extend automatically to this more general situation.

The boundary conditions

We denote $\partial_i\Omega_0 = \Gamma_i^- \cup \Gamma_i^+$ the boundary in x_i direction, $i \in \{1, 2\}$, see Figure 7.1,

$$\Gamma_1^\pm := \{\pm l\} \times J_2, \qquad \Gamma_2^\pm := J_1 \times \{\pm a\}. \tag{7.15}$$

Boundary conditions imposed respectively on $\partial_1\Omega_0$ and $\partial_2\Omega_0$ are of different nature. Having in mind the situation when Γ is a closed curve, standard periodic boundary conditions are imposed on $\partial_1\Omega_0$, *i.e.*,

$$\psi(-l, x_2) = \psi(l, x_2), \qquad \partial_1\psi(-l, x_2) = \partial_1\psi(l, x_2), \tag{7.16}$$

for a.e. $x_2 \in J_2$, where ψ denotes any function from the domain of H. We assume also the symmetry condition on the geometry

$$\boxed{\forall (x_1, x_2) \in \Omega_0 : \quad f(-l, x_2) = f(l, x_2),} \tag{7.17}$$

in order to have indeed periodic system in x_1 direction.

On the other hand, non-self-adjoint $\mathcal{PT}$-symmetric boundary conditions are imposed on $\partial_2\Omega_0$. A general form of $\mathcal{PT}$-symmetric boundary conditions was presented in [2]; further study and more general approach to extensions can be found in [4, 3]. Denoting

$$\Psi := \begin{pmatrix} \psi \\ \partial_2\psi \end{pmatrix}, \tag{7.18}$$

there are two types of the conditions, separated and connected.

I. separated:

$$\begin{pmatrix} \pm\beta(x_1) + \mathrm{i}\alpha(x_1) & 0 \\ 0 & 1 \end{pmatrix} \Psi(x_1, \pm a) = 0 \tag{7.19 I}$$

for a.e. $x_1 \in J_1$, with α, β being real-valued functions.

II. connected:

$$\Psi(x_1, a) = B(x_1)\Psi(x_1, -a), \tag{7.19 II}$$

for a.e. $x_1 \in J_1$, where the matrix B has the form

$$B(x_1) := \begin{pmatrix} \sqrt{1 + b(x_1)c(x_1)}\, e^{\mathrm{i}\phi(x_1)} & b(x_1) \\ c(x_1) & \sqrt{1 + b(x_1)c(x_1)}\, e^{-\mathrm{i}\phi(x_1)} \end{pmatrix}$$

with b, c, ϕ being real-valued functions satisfying $b > 0$, $c \geq -1/b$, $\phi \in [-\pi, \pi)$.

We specify assumptions on smoothness, boundedness and periodicity of the functions entering the boundary conditions later. The index $\iota \in \{\mathrm{I}, \mathrm{II}\}$ will be used throughout the paper to distinguish between the two types of boundary conditions.

The boundary conditions (7.19ι) are $\mathcal{PT}$-symmetric in following sense: if a function ψ satisfies (7.19ι), then the function $\mathcal{PT}\psi$ satisfies (7.19ι) as well. Here and in the sequel the symmetry operators $\mathcal{P}$ and $\mathcal{T}$ are defined as follows:

$$(\mathcal{P}\psi)(x_1, x_2) := \psi(x_1, -x_2), \qquad \mathcal{T}\psi := \overline{\psi}. \tag{7.20}$$

It is important to stress that the $\mathcal{PT}$-symmetric boundary conditions (7.19ι) do not automatically imply that the operator H is $\mathcal{PT}$-symmetric, unless additional assumption on the geometry of Ω_0 is imposed. The assumption, ensuring the $\mathcal{PT}$-symmetry of H (*cf* Proposition 7.1 below), reads

$$\boxed{\forall (x_1, x_2) \in \Omega_0 : \quad f(x_1, x_2) = f(x_1, -x_2).} \tag{7.21}$$

In view of (7.12), a necessary condition to satisfy the second requirement in (7.21) is that the curve Γ is a geodesic, *i.e.* $\kappa = 0$.

The functional spaces

The space in which we give a precise meaning of H is the Hilbert space $L^2(\Omega_0, G)$, *i.e.*, the class of all measurable functions φ, ψ on Ω_0 for which the norm $\|\cdot\|_G$ induced by the inner product

$$(\varphi, \psi)_G := \int_{\Omega_0} \overline{\varphi(x)}\, \psi(x)\; |G(x)|^{1/2}\, \mathrm{d}x \tag{7.22}$$

is finite. Assuming (7.14), the norm $\|\cdot\|_G$ in $L^2(\Omega_0, G)$ is equivalent to the usual one $\|\cdot\|$ in $L^2(\Omega_0)$. Moreover, the 'energy space'

$$W^{1,2}(\Omega_0, G) := \left\{\psi \in L^2(\Omega_0, G) \;\middle|\; |\nabla_G\psi|_G^2 := \overline{\partial_i\psi} G^{ij} \partial_j\psi \in L^2(\Omega_0, G)\right\} \tag{7.23}$$

can be as a vector space identified with the usual Sobolev space $W^{1,2}(\Omega_0)$.

However, this equivalence does not hold for $W^{2,2}$-spaces, unless one assumes extra regularity condition on f:

$$\boxed{\forall x_2 \in J_2 : \quad f(\cdot, x_2),\; f^{-1}(\cdot, x_2) \in W^{1,\infty}(J_1).} \tag{7.24}$$

Under this assumption, which is actually equivalent to the Lipschitz continuity of f, f^{-1} in the first argument (*cf* [20, Chapt. 5.8.2.b., Thm. 4]), one can indeed identify the $W^{2,2}$-Sobolev space on the Riemannian manifold (Ω_0, G) (precisely defined, *e.g.*, in [26, Sec. 2.2]) with the usual Sobolev space $W^{2,2}(\Omega_0)$.

The schism: two definitions of the Hamiltonian

Although the above equivalence of the $W^{2,2}$-spaces under the condition (7.24) is not explicitly used in this paper, it is in fact hidden in our proof that the particle Hamiltonian on $L^2(\Omega_0, G)$ naturally identified with

$$H_\iota \psi := -\Delta_G \psi, \tag{7.25a}$$

$$\psi \in \mathsf{D}(H_\iota) := \big\{\psi \in W^{2,2}(\Omega_0) \;\big|\; \psi \text{ satisfies (7.16) and (7.19}\iota)\big\}. \tag{7.25b}$$

is well defined (*cf* Theorem 7.1). As mentioned in Section 7.2.3, we use the notation H_ι, with $\iota \in \{\mathrm{I}, \mathrm{II}\}$, to distinguish between separated (7.19 I) and connected (7.19 II) boundary conditions.

To avoid the additional assumption (7.24), one can always interpret (7.13) in the weak sense of quadratic forms, which gives rise to an alternative Hamiltonian $\tilde{H}_\iota$ (*cf* Corollary 7.1). This is the content of the following section, where we also show that $H_\iota = \tilde{H}_\iota$ provided that (7.17), (7.24), and some analogous hypotheses about the boundary-coupling functions hold.

7.3 General properties

The main goal of this section is to show that the Hamiltonian H_ι introduced in (7.25) is a well defined operator, in particular that it is closed. This will be done by proving that $H_\iota = \tilde{H}_\iota$, where $\tilde{H}_\iota$ is the alternative operator defined through a closed quadratic form. Finally, we establish some general spectral properties of the Hamiltonians.

7.3.1 The Hamiltonian defined via quadratic form

Taking the sesquilinear form $(\varphi, H_\iota \psi)_G$ with $\varphi, \psi \in \mathsf{D}(H_\iota)$ and integrating by parts, one arrives to a sesquilinear form, which is well defined for a wider class of functions φ, ψ, not necessarily possessing second (weak) derivatives. The function f is assumed to satisfy (7.14) and (7.17), however the extra regularity condition (7.24) is *not* required.

More precisely, exclusively under assumption (7.14) for a moment, we define the sesquilinear form

$$h_\iota(\varphi,\psi) := h^1(\varphi,\psi) + h^2_\iota(\varphi,\psi),$$
$$\varphi,\psi \in \mathsf{D}(h_\iota) := W^{1,2}_{\mathrm{per}}(\Omega_0) \equiv \big\{\psi \in W^{1,2}(\Omega_0) \;\big|\; \psi(-l,x_2) = \psi(l,x_2)\big\}\,,$$

where, for any $\varphi,\psi \in \mathsf{D}(h_\iota)$,

$$\begin{aligned}
h^1(\varphi,\psi) \;&:=\; \big(f^{-1}\partial_1\varphi, f^{-1}\partial_1\psi\big)_G + \big(\partial_2\varphi,\partial_2\psi\big)_G\,,\\
h^2_{\mathrm{I}}(\varphi,\psi) \;&:=\; \big(\varphi,(\beta+\mathrm{i}\alpha)\psi\big)_G^{\Gamma_2^+} + \big(\varphi,(\beta-\mathrm{i}\alpha)\psi\big)_G^{\Gamma_2^-}\,,\\
h^2_{\mathrm{II}}(\varphi,\psi) \;&:=\; \big(\varphi,B_{12}^{-1}\mathcal{P}\psi\big)_G^{\Gamma_2^+} + \big(\varphi,B_{12}^{-1}\mathcal{P}\psi\big)_G^{\Gamma_2^-}\\
&\qquad -\big(\varphi,B_{22}B_{12}^{-1}\psi\big)_G^{\Gamma_2^+} - \big(\varphi,B_{11}B_{12}^{-1}\psi\big)_G^{\Gamma_2^-}\,.
\end{aligned}$$

Here B_{ij} denotes the elements of the matrix B defined in (7.19), the operator $\mathcal{P}$ is introduced in (7.20) and

$$(\varphi,\psi)_G^{\Gamma_2^\pm} := \int_{-l}^{l} \overline{\varphi(x_1,\pm a)}\,\psi(x_1,\pm a)\,f(x_1,\pm a)\,\mathrm{d}x_1.$$

All the boundary terms should be understood in sense of traces [1].

Lemma 7.1. *Let f satisfy* (7.14)*. The forms h_ι, h^1 are densely defined. h^1 is a symmetric, positive, closed form (associated to the self-adjoint Laplace-Beltrami operator in $L^2(\Omega_0, G)$ with periodic boundary conditions on $\partial_1\Omega_0$ and Neumann boundary conditions on $\partial_2\Omega_0$).*

Proof. The density of the domains is obvious, properties of h^1 are well known, see the detailed discussion on a similar problem in [15, Sect. 7.2]. □

Although the forms h_ι are not symmetric, we show that h^2_ι can be understood as small perturbations of h^1.

Lemma 7.2. *Let $b, 1/b, c, \alpha, \beta \in L^\infty(J_1)$ and let f satisfy* (7.14)*. Then h^2_ι are relatively bounded with respect to h^1 with*

$$|h^2_\iota[\psi]| \le \varepsilon\, h^1[\psi] + \varepsilon^{-1} C \|\psi\|^2_G, \tag{7.26}$$

for all $\psi \in W^{1,2}_{\mathrm{per}}(\Omega_0)$ and any positive number ε. The constant C depends on the function f, dimensions a, l, and boundary-coupling functions α, β or b, c, ϕ.

Proof. The proof is based on the estimate

$$\int_{-l}^{l} |\psi(x_1, \pm a)|^2 \, \mathrm{d}x_1 \leq \epsilon \, \|\nabla\psi\|^2 + \epsilon^{-1} \tilde{C} \, \|\psi\|^2, \tag{7.27}$$

where ϵ is an arbitrary positive constant and $\tilde{C}$ is a positive constant depending only on a and l. We give the proof for h_{I}^2 only because the other case is analogous. The assumptions on α, β and property (7.14) allow us to estimate the functions $|\alpha|, |\beta|$ and f by their L^∞-norms. Consequent application of (7.27) therefore yields

$$\left|h_{\mathrm{I}}^2[\psi]\right| \leq \epsilon \, \|f\|_{L^\infty(\Omega_0)} \|\nabla\psi\|^2 + \epsilon^{-1} 2 \, \tilde{C} \left(\|\alpha\|_{L^\infty(J_1)} + \|\beta\|_{L^\infty(J_1)}\right) \|f\|_{L^\infty(\Omega_0)} \, \|\psi\|^2.$$

In order to replace the term $\|\nabla\psi\|^2$ by $h^1[\psi]$, the regularity assumption on geometry (7.14) is used. Once we consider the equivalence of the norms $\|\cdot\|$ and $\|\cdot\|_G$ and the arbitrariness of ϵ, we obtain the estimate (7.26). □

Corollary 7.1. *Let $b, 1/b, c, \alpha, \beta \in L^\infty(J_1)$ and let f satisfy* (7.14). *Then there exist the unique m-sectorial operators $\tilde{H}_\iota$ in $L^2(\Omega_0, G)$ such that*

$$h_\iota(\varphi, \psi) =: (\varphi, \tilde{H}_\iota \psi)_G \tag{7.28}$$

for all $\psi \in \mathsf{D}(\tilde{H}_\iota)$ and $\varphi \in \mathsf{D}(h_\iota)$, where

$$\begin{aligned} \mathsf{D}(\tilde{H}_\iota) := \big\{\psi \in W^{1,2}_{\mathrm{per}}(\Omega_0) \quad \big| \quad & \exists F \in L^2(\Omega_0, G), \ \forall \varphi \in W^{1,2}_{\mathrm{per}}(\Omega_0), \\ & h_\iota(\varphi, \psi) = (\varphi, F)_G \big\}. \end{aligned} \tag{7.29}$$

Proof. With regard to Lemmata 7.1, 7.2, and the perturbation result [32, Thm. VI.3.4], the statement follows by the first representation theorem [32, Thm. VI.2.1]. □

7.3.2 The equivalence of the two definitions

Under stronger assumptions on smoothness of functions appearing in boundary conditions (7.19ι) and on the function f entering the metric tensor G, we show that operators $\tilde{H}_\iota$ associated to the forms h_ι are equal to the Hamiltonians H_ι defined in (7.25). To prove this, we need the following lemma. Let us introduce a space of Lipschitz continuous functions over $[-l, l]$ satisfying periodic boundary conditions:

$$W^{1,\infty}_{\mathrm{per}}(J_1) := \big\{\psi \in W^{1,\infty}(J_1) \,\big|\, \psi(-l) = \psi(l)\big\}.$$

Lemma 7.3. *Let $\alpha, \beta, b, 1/b, c, \phi \in W^{1,\infty}_{\mathrm{per}}(J_1)$ and let f satisfy* (7.14), (7.17), *and* (7.24). *Then for every $F \in L^2(\Omega_0, G)$, a solution ψ to the problem*

$$\forall \varphi \in W^{1,2}_{\mathrm{per}}(\Omega_0), \qquad h_\iota(\varphi, \psi) = (\varphi, F)_G \,, \tag{7.30}$$

belongs to $\mathsf{D}(H_\iota)$ introduced in (7.25b).

Proof. We prove the separated boundary conditions case only, the connected case is analogous. For each $\psi \in W^{1,2}_{\mathrm{per}}(\Omega_0)$ We introduce a difference quotient

$$\delta\psi(x_1, x_2) := \frac{\psi_\delta(x_1, x_2) - \psi(x_1, x_2)}{\delta}, \tag{7.31}$$

where $\psi_\delta(x_1, x_2) := \psi(x_1 + \delta, x_2)$ and δ is a small real number. The shifted value $\psi_\delta(x_1, x_2)$ is well defined for every $x_1 \in J_1$ and $\delta \in \mathbb{R}$ by extending ψ periodically to $\mathbb{R}$. We use periodic extensions of other functions in x_1 direction throughout the whole proof without further specific comments. The estimate

$$\|\delta\psi\| \leq \|\psi\|_{W^{1,2}(\Omega_0)} \tag{7.32}$$

is valid for δ small enough [20, Sec. 5.8.2., Thm. 3].

We express the difference of identities (7.30) for ψ and ψ_δ, whence we get for every $\varphi \in W^{1,2}_{\mathrm{per}}(\Omega_0)$

$$\begin{aligned} &\big(\partial_1\varphi, (\delta f^{-1})\partial_1\psi\big) + \big(\partial_1\varphi, f_\delta^{-1}\partial_1(\delta\psi)\big) + \big(\partial_2\varphi, (\delta f)\partial_2\psi\big) \\ &+ \big(\partial_2\varphi, f_\delta\partial_2(\delta\psi)\big) + \big(\varphi, \delta(f(\beta + \mathrm{i}\alpha))\psi_\delta\big)^{\Gamma_2^+} + \big(\varphi, f(\beta + \mathrm{i}\alpha)(\delta\psi)\big)^{\Gamma_2^+} \\ &+ \big(\varphi, \delta(f(\beta - \mathrm{i}\alpha))\psi_\delta\big)^{\Gamma_2^-} + \big(\varphi, f(\beta - \mathrm{i}\alpha)(\delta\psi)\big)^{\Gamma_2^-} \\ &= \big(\varphi, (\delta f)F_\delta\big) + \big(\varphi, f(\delta F)\big), \end{aligned} \tag{7.33}$$

where $(\cdot,\cdot)$ is the inner product in $L^2(\Omega_0)$ and

$$(\varphi,\psi)^{\Gamma_2^\pm} := \int_{-l}^{l} \overline{\varphi(x_1,\pm a)}\,\psi(x_1,\pm a)\,\mathrm{d}x_1. \tag{7.34}$$

We insert $\varphi = \delta\psi$ into equation (7.33) and apply the 'integration-by-parts' formula [20, Sec. 5.8.2] for difference quotients, *i.e.*, $(\varphi,\delta F\big) = -\big((-\delta)\varphi, F\big)$, in order to avoid the difference quotient of the arbitrary (*e.g.* possibly non-continuous) function $F \in L^2(\Omega_0, G)$. Using the embedding of $W^{1,2}(\Omega_0)$ in $L^2(\partial\Omega_0)$, the regularity assumptions on α, β and f, the Schwarz and Cauchy inequalities, and the estimate (7.32), we obtain

$$\|\delta\psi\|_{W^{1,2}(\Omega_0)} \leq C, \tag{7.35}$$

where C is a constant independent of δ. By standard arguments [20, D.4], this estimate yields that $\partial_1\psi \in W^{1,2}(\Omega_0)$.

At the same time, standard elliptic regularity theory [23, Thm. 8.8] implies that the solution ψ to (7.30) belongs to $W^{2,2}_{\mathrm{loc}}(\Omega_0)$. Thus ψ satisfies the equation

$$-\Delta_G\psi = F \tag{7.36}$$

a.e. in Ω_0. If we express $\partial_2^2\psi$ from (7.36), we obtain that $\partial_2^2\psi \in L^2(\Omega_0)$.

It remains to check boundary conditions of $\mathsf{D}(H_{\mathrm{I}})$. Once the $W^{2,2}$-regularity of the solution ψ is established, this can be done by using integration by parts in the identity (7.30) and considering the arbitrariness of φ, see [10, Lemma 3.2] for the more detailed discussion in an analogous situation. □

Let us write $H_{\mathrm{I}}(\alpha,\beta)$ and $H_{\mathrm{II}}(b,c,\phi)$ if we want to stress the dependence of the Hamiltonians on functions α,β and b,c,ϕ entering the boundary conditions.

Theorem 7.1. *Let $\alpha,\beta,b,1/b,c,\phi \in W^{1,\infty}_{\mathrm{per}}(J_1)$ and let f satisfy* (7.14), (7.17), *and* (7.24). *Then*

1. $\tilde{H}_\iota = H_\iota$,
2. *H_ι are m-sectorial operators,*
3. *the adjoint operators H_ι^* can be found as*

$$H_{\mathrm{I}}^*(\alpha,\beta) = H_{\mathrm{I}}(-\alpha,\beta), \qquad H_{\mathrm{II}}^*(b,c,\phi) = H_{\mathrm{II}}(b,c,-\phi),$$

4. *the resolvents of H_ι are compact.*

Proof. Ad 1. It is easy to verify, by integration by parts, that if $\psi \in \mathsf{D}(H_\iota)$ then $\psi \in \mathsf{D}(\tilde{H}_\iota)$; in fact, the function F from (7.29) satisfies $F = -\Delta_G\psi$ in the distributional sense. Thus $H_\iota \subset \tilde{H}_\iota$. The more non-trivial inclusion $\tilde{H}_\iota \subset H_\iota$ follows from Lemma 7.3. Once the equality of the operators is established, the other properties readily follow from the corresponding properties for $\tilde{H}_\iota$.

Ad 2. $\tilde{H}_\iota$ is m-sectorial by Corollary 7.1.

Ad 3. By [32, Thm. VI.2.5], the adjoint operator $\tilde{H}_\iota^*$ is associated to the adjoint form $h_\iota^*(\varphi,\psi) := \overline{h_\iota(\psi,\varphi)}$, which establishes the required identities for $\tilde{H}_\iota$.

Ad 4. The compactness of the resolvents for $\tilde{H}_\iota$ is provided by the perturbation result [32, Thm. VI.3.4] and Lemmata 7.1, 7.2. □

7.3.3 Spectral consequences

Since the Hamiltonians H_ι are m-sectorial by Theorem 7.1, the spectrum (as a subset of the numerical range) is contained in a sector of the complex plane, *i.e.*, there exists a vertex $\gamma \in \mathbb{R}$ and a semi-angle $\theta \in [0,\pi/2)$ such that

$$\sigma(H_\iota) \subset \big\{\zeta \in \mathbb{C} \;\big|\; |\arg(\zeta-\gamma)| \leq \theta\big\}.$$

Furthermore, since the resolvents of H_ι are compact, the spectra of H_ι are purely discrete, as it is reasonable to expect for the Laplacian defined on a bounded manifold.

Under the additional assumptions on the geometry of the model (7.21), one can show that H_ι are $\mathcal{PT}$-symmetric.

Proposition 7.1. *Let $\alpha,\beta,b,1/b,c,\phi \in W^{1,\infty}_{\mathrm{per}}(J_1)$ and let f satisfy* (7.14), (7.21), *and* (7.24). *Then Hamiltonians H_ι are*

1. *$\mathcal{PT}$-symmetric,* i.e., $(\mathcal{PT})H_\iota \subset H_\iota(\mathcal{PT})$,

2. *$\mathcal{P}$-pseudo-Hermitian,* i.e., $H_\iota = \mathcal{P}H_\iota^*\mathcal{P}$,

3. *$\mathcal{T}$-self-adjoint,* i.e., $H_\iota = \mathcal{T}H_\iota^*\mathcal{T}$,

where the operators $\mathcal{P}$ and $\mathcal{T}$ are defined in (7.20).

Proof. Note that the $\mathcal{PT}$-symmetry relation means that whenever $\psi \in \mathsf{D}(H_\iota)$, $\mathcal{PT}\psi$ also belongs to $\mathsf{D}(H_\iota)$ and $\mathcal{PT}H_\iota\psi = H_\iota\mathcal{PT}\psi$. This can be verified directly using the definition of H_ι via (7.25). The proofs of the remaining statements are based on the explicit knowledge of the adjoint operators, Theorem 7.1.3. □

Corollary 7.2. *Under the hypotheses of Proposition 7.1, the spectra of H_ι are invariant under complex conjugation,* i.e.,

$$\forall\lambda \in \mathbb{C}\,, \qquad \lambda \in \sigma(H_\iota) \Longleftrightarrow \overline{\lambda} \in \sigma(H_\iota)\,.$$

Proof. Recall that the spectrum of H_ι is purely discrete due to Theorem 7.1.4. With regard to $\mathcal{PT}$-symmetry, it is easy to check that if ψ is the eigenfunction corresponding to the eigenvalue λ, then $\mathcal{PT}\psi$ is the eigenfunction corresponding to the eigenvalue $\overline{\lambda}$. □

7.4 Solvable models: constantly curved manifolds

In order to examine basic effects of curvature on the spectrum of the Hamiltonians we investigate solvable models now. We restrict ourselves to the spectral problem in constantly curved manifolds and subjected to constant interactions on the boundary, *i.e.*, the functions $K, \alpha, \beta, b, c, \phi$ are assumed to be constant. Moreover, we assume that Γ is a geodesic, *i.e.* $\kappa = 0$, to have (7.21).

7.4.1 Preliminaries

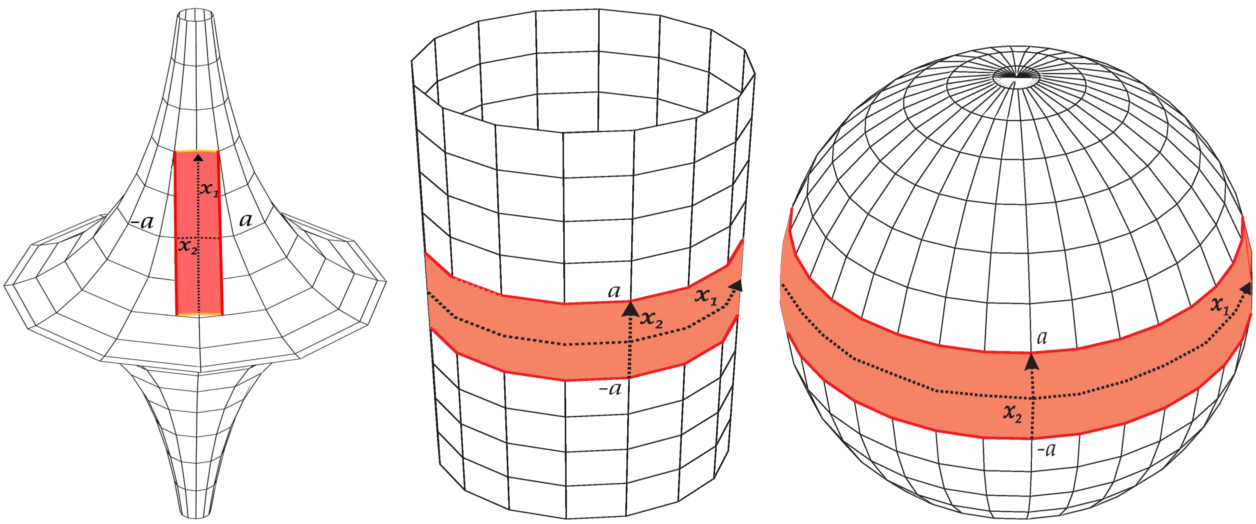
To emphasize the dependence of the Hamiltonians H_ι on the curvature K, we use the notation $H_{\iota(K)}$ in this section. One can easily derive the scaling properties of eigenvalues for constant $K \neq 0$:

$$\lambda_\iota(K, a, l) \;=\; |K|\,\lambda_\iota\big(\pm 1, \sqrt{|K|}\,a, \sqrt{|K|}\,l\big).$$

Hence, the decisive factor for qualitative properties of the spectrum is the sign of K, while the specific value of curvature is not essential. Hereafter we restrict ourselves to

$$K \in \{-1, 0, 1\}\,. \tag{7.37}$$

Possible realizations of the ambient manifolds $\mathcal{A}$ corresponding to these three cases are pseudosphere, cylinder, and sphere, respectively, see Figure 7.2.



(a) $K = -1$, pseudosphere (b) $K = 0$, cylinder (c) $K = 1$, sphere

Figure 7.2: Realizations of the constantly curved manifolds.

Remark 7.2. The pseudosphere should be considered as a useful realization of $\mathcal{A}$ with $K = -1$ only locally, since no complete surface of constant negative curvature can be globally embedded in $\mathbb{R}^3$ (this is reflected by the singular equator in Figure 7.2.(a)). However, since Ω is a precompact subset of $\mathcal{A}$, the incompleteness of the pseudosphere is not a real obstacle here.

Moreover, hereafter we put $l = \pi$, so that the length of the strip is 2π. This provides an instructive visualization of Ω as a tubular neighbourhood of a geodesic circle on the cylinder and the sphere, see Figure 7.2.

For $\kappa = 0$ and constant curvatures (7.37), the Jacobi equation (7.12) admits the explicit solutions

$$f_{(K)}(x_1, x_2) = \begin{cases} \cosh x_2 & \text{if} \quad K = -1\,, \\ 1 & \text{if} \quad K = 0\,, \\ \cos x_2 & \text{if} \quad K = 1\,. \end{cases} \tag{7.38}$$

It follows that the assumption (7.14) is satisfied for any positive a if $K = -1, 0$, while one has to restrict to $a < \pi/2$ if $K = 1$. The latter is also sufficient to satisfy (7.10) for the sphere. There is no restriction on a to have (7.10) if Γ is the geodesic circle on the cylinder. In any case (including the pseudosphere), (7.10) can be always satisfied for sufficiently small a. The other hypotheses, *i.e.* (7.17), (7.21), and (7.24), clearly hold regardless of the curvature sign.

Remark 7.3. In view of Remark 7.1, $a < \pi/2$ for $K = 1$ is the only essential restriction in the constant-curvature case (7.38).

Explicit structures of the Hamiltonians $H_{\iota(K)}$ introduced in (7.25) readily follow from (7.13) by using (7.38):

$$H_{\iota(K)} = \begin{cases} -\dfrac{1}{\cosh^2 x_2}\partial_1^2 - \dfrac{1}{\cosh x_2}\partial_2 \cosh x_2 \partial_2 & \text{if} \quad K = -1\,, \\ -\partial_1^2 - \partial_2^2 & \text{if} \quad K = 0\,, \\ -\dfrac{1}{\cos^2 x_2}\partial_1^2 - \dfrac{1}{\cos x_2}\partial_2 \cos x_2 \partial_2 & \text{if} \quad K = 1\,, \end{cases} \tag{7.39}$$

on $\mathsf{D}(H_{\iota(K)})$.

7.4.2 Partial wave decomposition

Since both the coefficients of $H_{\iota(K)}$ and the boundary conditions are independent of the first variable x_1, we can decompose the Hamiltonians into a direct sum of transverse one-dimensional operators. The decomposition is based on the following lemma.

Lemma 7.4.

$$\forall \Psi \in L^2(\Omega_0, G), \qquad \Psi(x_1, x_2) = \sum_{m\in\mathbb{Z}} \psi_m(x_2)\phi_m(x_1) \quad \text{in} \quad L^2(\Omega_0, G), \tag{7.40}$$

where

$$\phi_m(x_1) := \frac{1}{\sqrt{2\pi}} e^{imx_1}, \qquad \psi_m(x_2) := \big(\phi_m, \Psi(\cdot, x_2)\big)_{L^2(J_1)}. \tag{7.41}$$

Proof. We may restrict the proof to $L^2(\Omega_0)$ only because the norms $\|\cdot\|$ and $\|\cdot\|_G$ are equivalent due to (7.14). Let us also stress that G is independent of x_1 and $\{\phi_m\}_{m\in\mathbb{Z}}$ forms an orthonormal basis of $L^2(J_1)$. Hence

$$\left\| \sum_{m\in\mathbb{Z}} \psi_m(x_2)\phi_m \right\|_{L^2(J_1)} = \|\Psi(\cdot, x_2)\|_{L^2(J_1)} \in L^2(J_2). \tag{7.42}$$

The decomposition in $L^2(\Omega_0)$ can be then justified by using the dominated convergence theorem. □

Writing $\Psi(x_1, x_2) = \sum_{m\in\mathbb{Z}} \phi_m(x_1)\psi_m(x_2)$ in the expression $H_{\iota(K)}\Psi$ and formally interchanging the summation and differentiation, we (formally) arrive at the decomposition:

$$H_{\iota(K)} = \bigoplus_{m\in\mathbb{Z}} H_{\iota(K)}^m B^m \tag{7.43}$$

with

$$H^m_{\iota(K)} := \begin{cases} -\dfrac{1}{\cosh x_2}\partial_2 \cosh x_2\, \partial_2 + \dfrac{m^2}{\cosh^2 x_2} & \text{if} \quad K=-1\,, \\ -\partial_2^2 + m^2 & \text{if} \quad K=0\,, \\ -\dfrac{1}{\cos x_2}\partial_2 \cos x_2\, \partial_2 + \dfrac{m^2}{\cos^2 x_2} & \text{if} \quad K=1\,, \end{cases}$$

where B^m are bounded rank-one operators defined by

$$(B^m\Psi)(x_1,x_2) := \big(\phi_m, \Psi(\cdot,x_2)\big)_{L^2(J_1)}\,\phi_m(x_1)\,. \tag{7.44}$$

The operators $H^m_{\iota(K)}$ act in $L^2(J_2, \mathrm{d}\nu_{(K)})$ spaces with the measure

$$\mathrm{d}\nu_{(K)}(x_2) := \begin{cases} \cosh x_2\, \mathrm{d}x_2 & \text{if} \quad K=-1\,, \\ \mathrm{d}x_2 & \text{if} \quad K=0\,, \\ \cos x_2\,\mathrm{d}x_2 & \text{if} \quad K=1\,. \end{cases} \tag{7.45}$$

The domains of $H^m_{\iota(K)}$ are given by

$$\mathsf{D}(H^m_{\iota(K)}) := \big\{\psi \in W^{2,2}(J_2) \;\big|\; \psi \text{ satisfies } (7.19\iota)\big\}, \tag{7.46}$$

with obvious modification of the $\mathcal{PT}$-symmetric boundary conditions (7.19ι) to the one-dimensional situation.

To justify the decomposition (7.43) in a resolvent sense, we need the following technical lemma specifying the numerical range of $H^m_{\iota(K)}$.

Lemma 7.5. *Let $\Xi^m_{\iota(K)}$ denote the numerical range of $H^m_{\iota(K)}$. Then there exist real constants c_0, c_1 independent of $m \neq 0$ such that*

$$\Xi^m_{\iota(K)} \subset \Big\{z\in\mathbb{C} \;\Big|\; \Re z \geq c_0 + m^2,\ |\Im z| \leq c_1\sqrt{\Re z + |c_0| - m^2}\Big\}\,. \tag{7.47}$$

Proof. We give the proof for $H^m_{\mathrm{I}(+1)}$ only, the other cases are analogous. We abbreviate $(\cdot,\cdot)_+ := (\cdot,\cdot)_{L^2(J_2,\mathrm{d}\nu_{(+1)})}$ and define

$$v^m(x_2) := \frac{m^2}{\cos^2 x_2}\,, \qquad h[\psi] := \big(\psi, H^m_{\mathrm{I}(+1)}\psi\big)_+\,,$$

for every $\psi \in \mathsf{D}(H^m_{\mathrm{I}(+1)})$. Integration by parts yields the following expressions for real and imaginary parts of $h[\psi]$:

$$\begin{aligned} \Re h[\psi] &= \|\psi'\|_+^2 + (\psi, v^m\psi)_+ + \beta\cos a\left(|\psi(a)|^2 + |\psi(-a)|^2\right), \\ \Im h[\psi] &= \alpha\cos a\big(|\psi(a)|^2 - |\psi(-a)|^2\big), \end{aligned}$$

for every $\psi \in \mathsf{D}(H^m_{\mathrm{I}(+1)})$. The estimates of $\Re h[\psi]$ and $\Im h[\psi]$ can be easily obtained taking into account the equivalence of the norm $\|\cdot\|_{L^2(J_2)}$ with $\|\cdot\|_+$ and using the one-dimensional version of the estimate (7.27). □

Now we are in a position to establish the main result of this subsection.

Proposition 7.2. *$D := \bigcap_{m\in\mathbb{Z}} \varrho\left(H^m_{\iota(K)}\right)$ is non-empty and $D \subset \varrho\left(H_{\iota(K)}\right)$. For every $z \in D$,*

$$(H_{\iota(K)} - z)^{-1} = \bigoplus_{m\in\mathbb{Z}} \big(H^m_{\iota(K)} - z\big)^{-1} B^m, \tag{7.48}$$

where $(H^m_{\iota(K)} - z)^{-1}$ abbreviates $1 \otimes (H^m_{\iota(K)} - z)^{-1}$ acting on $L^2(J_1) \otimes L^2(J_2, \mathrm{d}\nu_{(K)})$ and B^m are defined in (7.44).

Proof. We give a proof for $H^m_{\mathrm{I}(+1)}$ only, the remaining cases are analogous. Take $z \in D$, for every $\Psi \in L^2(\Omega, G)$ and $m \in \mathbb{Z}$, we define

$$U_m(x_2) := \big(H^m_{\mathrm{I}(+1)} - z\big)^{-1}\psi_m(x_2), \tag{7.49}$$

where ψ_m was introduced in (7.41). It is clear that $U_m \in L^2(J_2, \mathrm{d}\nu_{(+1)})$. With regard to Lemma 7.5, take $m_0 \in \mathbb{Z}$ such that for every $m > m_0$, $z \notin \Xi^m_{\iota(K)}$. Using [32, Thm. V.2.3] together with Lemma 7.5, we get for $m > m_0$

$$\|U_m\|_{L^2(J_2)} \leq C_1 \frac{\|\psi_m\|_{L^2(J_2)}}{m^2+1}, \tag{7.50}$$

where C_1 is a constant independent of m, nonetheless depending on $z, |\alpha|, |\beta|$, and a. Let us remark that since $z \in D$, $\|U_m\|_{L^2(J_2)}$ are bounded for finitely many m smaller than m_0. From the identity

$$\|U_m'\|_+^2 + (-\mathrm{i}\alpha + \beta)\cos a|U_m(a)|^2 + (-\mathrm{i}\alpha - \beta)\cos a|U_m(-a)|^2 \\ +(v^m U_m, U_m)_+ - \overline{z}\|U_m\|_+^2 = (\psi_m, U_m)_+ ,$$

with v^m and $(\cdot,\cdot)_+$ defined in Lemma 7.5, we obtain the estimate for the norm of U_m' for $m > m_0$,

$$\|U_m'\|_{L^2(J_2)} \leq C_1 \frac{\|\psi_m\|_{L^2(J_2)}}{\sqrt{m^2+1}} \tag{7.51}$$

Again, for finitely many $m \leq m_0$, $\|U_m'\|_{L^2(J_2)}$ are clearly bounded. With regard to (7.42), (7.50), and (7.51), every function $R_m(x_1,x_2) := \phi_m(x_1)U_m(x_2)$ belongs to $W^{1,2}_{\mathrm{per}}(\Omega_0)$.

Our goal is to show that $R := \sum_{m\in\mathbb{Z}} R_m$ is in $W^{1,2}_{\mathrm{per}}(\Omega_0)$ as well.

The finite number of bounded terms with $m \leq m_0$ is included in the following estimates and equalities without any other specific comments. The identity (7.42) and inequality (7.50) together with Fubini's theorem imply

$$\left\|\sum_{m\in\mathbb{Z}} R_m\right\| \leq C_2\|\Psi\|.$$

A similar estimate can be obtained for $\partial_2 R_m$ provided that we use the inequality (7.51). For $\partial_1 R_m$, we have

$$\left\|\sum_{m=-N}^{N} \partial_1 R_m\right\|^2 = \sum_{m=-N}^{N} m^2\|U_m\|^2_{L^2(J_2)} \leq C_1^2 \sum_{m=-N}^{N} \frac{m^2}{m^2+1}\|\psi_m\|^2_{L^2(J_2)},$$

where we used the inequality (7.50). The fraction in the sum on the right hand side is bounded, therefore, using the Parseval equality, the limit $\sum_{m\in\mathbb{Z}} \partial_1 R_m$ remains in $L^2(\Omega_0)$. We conclude that R belongs to $W^{1,2}(\Omega_0)$ and

$$\|R\|_{W^{1,2}(\Omega_0)} \leq C_3\|\Psi\|_{L^2(\Omega_0)}.$$

It remains to verify that R belongs to $W^{1,2}_{\mathrm{per}}(\Omega_0)$. We introduce the partial sum $R_N := \sum_{m=-N}^{N} R_m$. The fact that $R_N \in W^{1,2}_{\mathrm{per}}(\Omega_0)$ for every $N \in \mathbb{N}$ and the (trace) embedding of $W^{1,2}(\Omega_0)$ in $L^2(\partial\Omega_0)$ yields

$$\left|\big(\varphi, R(-l,\cdot) - R(l,\cdot)\big)_+\right| = \left|\big(\varphi, R(-l,\cdot) - R_N(-l,\cdot) + R_N(-l,\cdot) - R(l,\cdot)\big)_+\right| \\ \leq 2\, C_4\, \|\varphi\|_+ \, \|R - R_N\|_{W^{1,2}(\Omega_0)}$$

for every $\varphi \in L^2(J_2, \mathrm{d}\nu_{(+1)})$; C_4 is a constant depending only on Ω_0. Notice that the left hand side does not depend on N. Hence, the periodicity of R is justified by taking the limit $N \to +\infty$ and considering the arbitrariness of φ.

Now, knowing that R belongs to $W^{1,2}_{\mathrm{per}}(\Omega_0)$, one can easily check that

$$\forall \varphi \in W^{1,2}_{\mathrm{per}}(\Omega_0)\,, \qquad h_{\mathrm{I}}(\varphi, R) - z(\varphi, R)_{L^2(\Omega_0,G)} = (\varphi, \Psi)_{L^2(\Omega_0,G)}\,.$$

This implies that $R \in \mathsf{D}(H_{\mathrm{I}(+1)})$, see Lemma 7.3, and $(H_{\mathrm{I}(+1)} - z)R = \Psi$. ☐

Proposition 7.2 has the important consequence for the spectrum of $H_{\iota(K)}$.

Corollary 7.3.

$$\sigma\big(H_{\iota(K)}\big) = \bigcup_{m\in\mathbb{Z}} \sigma\big(H^m_{\iota(K)}\big)$$

Proof. Resolvents on both sides of (7.48) are compact. The inclusion $\sigma\big(H_{\iota(K)}\big) \subset \cup_{m\in\mathbb{Z}}\sigma\big(H^m_{\iota(K)}\big)$ is proved (formulated for resolvent sets) in Proposition 7.2. The other inclusion is trivial since the existence of an eigenfunction ξ_{m_0} of $H^{m_0}_{\iota(K)}$ corresponding to an eigenvalue λ_0 implies that $\xi_{m_0}(x_2)\phi_{m_0}(x_1)$ is an eigenfunction of $H_{\iota(K)}$ corresponding to the same eigenvalue. ☐

Remark 7.4. Notice that the statement of Corollary 7.3 relating the spectra of a direct sum of operators with their individual spectra does not hold in general (*cf* [17, Thm. 8.1.12]). In our case, however, we have been able to prove the result due to the compactness of resolvents and additional information about the behaviour of the numerical ranges of $H^m_{\iota(K)}$ (*cf* Lemma 7.5).

7.4.3 Similarity to self-adjoint or normal operators

We proceed with an analysis of $H^m_{\iota(K)}$. For sake of simplicity, we drop the subscript 2 of the x_2 variable in the sequel. We remark that $\mathcal{PT}$-symmetry and $\mathcal{P}$-pseudo-Hermiticity of $H^m_{\iota(K)}$ is preserved with $\mathcal{P}$ and $\mathcal{T}$ being naturally restricted to $L^2(J_2, \mathrm{d}\nu_{(K)})$.

The operators $H^m_{\iota(K)}$ are neither self-adjoint nor normal, nevertheless we can show the following general result:

Theorem 7.2. *For every $m \in \mathbb{Z}$ and $K \in \{-1, 0, 1\}$:*

1. *The families of operators $H^m_{\mathrm{I}(K)}(\alpha, \beta)$, $H^m_{\mathrm{II}(K)}(b, c, \phi)$ are holomorphic with respect to parameters α, β, and b, c, ϕ entering the boundary conditions.*
2. *The spectrum of $H^m_{\iota(K)}$ is discrete consisting of simple eigenvalues (*i.e.*, the algebraic multiplicity being one), except of finitely many eigenvalues of algebraic multiplicity two and geometric multiplicity one that can appear for particular values of α, β and b, c, ϕ.*
3. *If all the eigenvalues are simple, then*
   a) *the eigenvectors of $H^m_{\iota(K)}$ form a Riesz basis in $L^2(J_2, \mathrm{d}\nu_{(K)})$,*
   b) *$H^m_{\iota(K)}$ is similar to a normal operator,* i.e., *for every m there exists a bounded operator ϱ with bounded inverse such that $\varrho H^m_{\iota(K)} \varrho^{-1}$ is normal,*
   c) *if moreover all eigenvalues are real, then $H^m_{\iota(K)}$ is similar to a self-adjoint operator,* i.e., *$\varrho H^m_{\iota(K)} \varrho^{-1}$ is self-adjoint.*
4. *Let us denote by $\{\psi_{i,m}\}_{i\in\mathbb{N}}$ the eigenfunctions of $H^m_{\iota(K)}$. The set of eigenfunctions $\mathscr{B} := \{\phi_m \psi_{i,m}\}_{m\in\mathbb{Z}, i\in\mathbb{N}}$, where ϕ_m were introduced in* (7.41)*, forms a Riesz basis of $L^2(\Omega_0, G)$.*

Remark 7.5. We remark that while each $H^m_{\iota(K)}$ is similar to a normal (or self-adjoint) operator, the similarity transformation ρ depends on m and there is *a priori* no uniform (in m) bound on ρ and ρ^{-1}.

Proof. Ad 1. In view of [32, Sect. VII, Ex. 1.15], the Hamiltonians $H^m_{\mathrm{I}(K)}(\alpha, \beta)$, considered as a family of operators depending on parameters α, β entering boundary conditions, are holomorphic. The same is true for $H^m_{\mathrm{II}(K)}(b, c, \phi)$.

Ad 2. The separated boundary conditions belong to the class of strongly regular boundary conditions [46, 47]. The connected $\mathcal{PT}$-symmetric boundary conditions are strongly regular as well because $\theta_1 = -b$, $\theta_{-1} = b$ (in Naimark's notation) and b is non-zero by the assumption in (7.19). Moreover, all the eigenvalues are simple [40] up to finitely many degeneracies that can appear: eigenvalues with algebraic multiplicity two and geometric multiplicity one.

Ad 3. With regard to the strong regularity of boundary conditions, the eigenfunctions of the Hamiltonian $H^m_{\iota(K)}$ form a Riesz basis [40], except the situations when the degeneracies appear. The existence of Riesz basis implies the similarity to a normal operator and as a special case the similarity to a self-adjoint operator if the spectrum of $H^m_{\iota(K)}$ is real.

In more details, let $\{\psi_n\}_{n\in\mathbb{N}}$ be the Riesz basis of eigenvectors of $H^m_{\iota(K)}$, *i.e.*, $H^m_{\iota(K)}\psi_n = \lambda_n \psi_n$. By definition, there exists a bounded operator ρ with bounded inverse such that $\{\rho\psi_n\}_{n\in\mathbb{N}}$ is an orthonormal basis that we denote by $\{e_n\}_{n\in\mathbb{N}}$. Then

$$\rho H^m_{\iota(K)} \rho^{-1} = \sum_{n\in\mathbb{N}} \lambda_n \, e_n (e_n, \cdot)_{L^2(\Omega_0, G)}$$

is a normal (self-adjoint if every $\lambda_n \in \mathbb{R}$) operator.

Ad 4. At first we show that $\mathscr{B}$ is complete, *i.e.*, $\mathscr{B}^\perp = \{0\}$. Take $\omega \in \mathscr{B}^\perp$, *i.e.*, for every $m \in \mathbb{Z}$, $i \in \mathbb{N}$,

$$\begin{aligned} 0 &= \int_{\Omega_0} \overline{\phi_m(x_1)\psi_{i,m}(x_2)} \omega(x_1, x_2) \mathrm{d}x_1 \mathrm{d}\nu_{(K)}(x_2) \\ &= \int_{J_2} \overline{\psi_{i,m}} \omega_m(x_2) \mathrm{d}\nu_{(K)}(x_2), \end{aligned}$$

where $\omega_m(x_2) := \displaystyle\int_{J_1} \overline{\phi_m(x_1)} \omega(x_1, x_2) \mathrm{d}x_1$. Since $\{\psi_{i,m}\}_{i\in\mathbb{N}}$ forms a Riesz basis, $\omega_m = 0$ a.e. in $L^2(J_2, \mathrm{d}\nu_{(K)})$ for every $m \in \mathbb{Z}$. Since $\{\phi_m\}_{m\in\mathbb{Z}}$ is the orthonormal basis of $L^2(J_1)$, $\omega = 0$ in $L^2(\Omega_0, G)$.

Now we define an involution $(\mathcal{P}_1\psi)(x_1, x_2) := \psi(-x_1, x_2)$. We show that $\psi_{i,m}$ can be normalized in such way that $\mathscr{B}$ is $\mathcal{P}_1\mathcal{T}$-orthonormal, *i.e.*,

$$\left(\phi_m\psi_{i,m}, \mathcal{P}_1\mathcal{T}\phi_n\psi_{j,n}\right)_{L^2(\Omega_0,G)} = \delta_{ij}\delta_{mn}.$$

Since $\mathcal{P}_1\mathcal{T}\phi_m = \phi_m$, $\mathcal{P}_1\mathcal{T}$-orthogonality follows immediately for $m \neq n$ because ϕ_m are orthonormal in $(\cdot,\cdot)_{L^2(J_1)}$ and G is independent of x_1. For $m = n$ we have

$$\left(\phi_m\psi_{i,m}, \mathcal{P}_1\mathcal{T}\phi_m\psi_{j,m}\right)_{L^2(\Omega_0,G)} = \left(\psi_{i,m}, \mathcal{T}\psi_{j,m}\right)_{L^2(J_2,\mathrm{d}\nu_{(K)})}. \tag{7.52}$$

If $i \neq j$, then the right hand side of (7.52) is zero because $\mathcal{T}\psi_{j,m}$ is an eigenfunction of $\left(H^m_{\iota(K)}\right)^*$. Indeed, it is a general fact that eigenfunctions of H and H^* corresponding to different eigenvalues are orthogonal. It remains to verify that if $i = j$, then the right hand side of (7.52) does not vanish, *i.e.*,

$$\int_{J_2} \psi^2_{j,m}(x_2)\,\mathrm{d}\nu_{(K)}(x_2) \neq 0.$$

However, this is precisely the condition on $\lambda_{j,m}$ being a simple eigenvalue of $H^m_{\iota(K)}$. It can be easily seen either directly or it follows from [22, Thm. 5]. □

Remark 7.6. Notice that an additional symmetry with respect to $\mathcal{P}_1$ was essential in the proof. The set of eigenfunctions $\mathscr{B}$ is not $\mathcal{T}$-orthonormal because the products $\left(\phi_m\psi_{i,m}, \mathcal{T}\phi_m\psi_{i,m}\right)_{L^2(\Omega_0,G)}$ vanish. This situation is typical for $\mathcal{T}$-self-adjoint operators with eigenvalues that are not simple [22].

7.4.4 Separated boundary conditions

At first, we investigate the Hamiltonians $H^m_{\mathrm{I}(0)}(\alpha,\beta)$. Then $H^m_{\mathrm{I}(\pm1)}(\alpha,0)$ are analysed. These results together allow us to describe the remaining $\beta \neq 0$ case.

Zero curvature

As expected, the zero curvature case is the simplest and it will serve as a reference model. In fact, the corresponding one-dimensional eigenvalue problem

$$\begin{cases} -\psi'' + m^2\psi = k^2\psi \quad \text{in} \quad (-a,a), \\ \psi'(\pm a) + (\mathrm{i}\alpha \pm \beta)\,\psi(\pm a) = 0, \end{cases} \tag{7.53}$$

has been already studied previously in [37]. Here we overtake the main results.

Proposition 7.3. *The spectrum of $H^m_{\mathrm{I}(0)}(\alpha,0)$ is real for all $m \in \mathbb{Z}$. The eigenvalues $\lambda_{j,m}$ and eigenfunctions $\psi_{j,m}$ can be written in the following form, $m \in \mathbb{Z}$,*

$$\lambda_{j,m} = \begin{cases} \alpha^2 + m^2 & \text{if} \quad j = 0\,, \\ k_j^2 + m^2 & \text{if} \quad j \geq 1\,, \end{cases} \tag{7.54}$$

$$\psi_{j,m}(x) = \begin{cases} C_0 \, \exp(-\mathrm{i}\alpha x) & \text{if } j = 0\,, \\ C_j \left(\cos(k_j x) + \dfrac{k_j \sin(k_j a) - \mathrm{i}\alpha\cos(k_j a)}{k_j\cos(k_j a) + \mathrm{i}\alpha\sin(k_j a)} \sin(k_j x) \right) & \text{if } j \geq 1, \end{cases}$$

where $k_j := \frac{j\pi}{2a}$. If $\alpha^2 \neq k_j^2$, i.e.*, there is no level-crossing for the same m, then the operator is similar to a self-adjoint operator or, equivalently, it is quasi-Hermitian.*

Remark 7.7. Closed formulae for the metric operator Θ for $H^m_{\mathrm{I}(0)}(\alpha,0)$ are presented in [37, 36]. The similarity transformation ϱ can be found as $\varrho = \sqrt{\Theta}$ or as any other decomposition of the positive operator $\Theta = \varrho^*\varrho$.

The α-dependence of eigenvalues λ for $m = 0, 1, 2$ is plotted in Figure 7.3.

The case of $\beta \neq 0$ is more complicated and as it was remarked in [37], the spectrum of $H^m_{\mathrm{I}(0)}(\alpha,\beta)$ can be complex. More precise results follow from a further analysis, not presented in [37].

Proposition 7.4.

1. *If $\beta > 0$, then the spectrum of $H^m_{\mathrm{I}(0)}(\alpha,\beta)$ is purely real for all $m \in \mathbb{Z}$ and $\alpha \in \mathbb{R}$.*

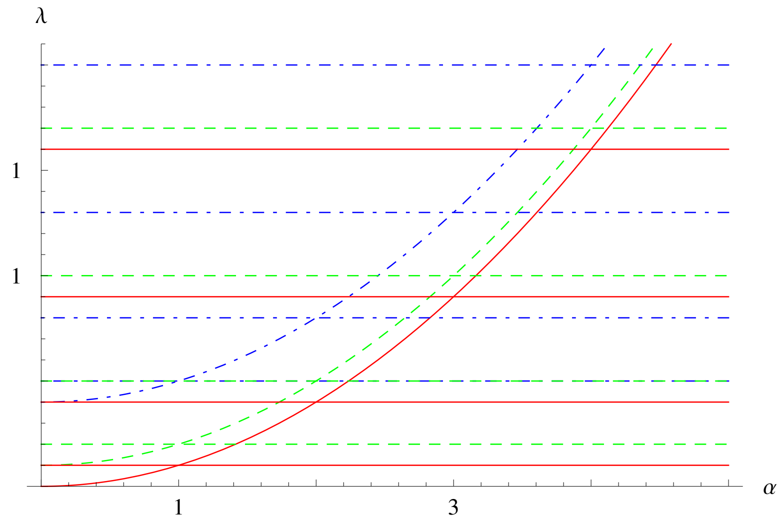


Figure 7.3: α-dependence of eigenvalues, zero curvature, $a = \pi/4$. Red (full), green (dashed), and blue (dot-dashed) curves correspond to $m = 0, 1, 2$ respectively.

2. *If $\beta < 0$, then the spectrum of $H^0_{\mathrm{I}(0)}(\alpha, \beta)$ is either purely real or there is one pair of complex conjugated eigenvalues with real part located in the neighbourhood of $\alpha^2+\beta^2$. For fixed negative β, the points α_n where a pair of complex conjugated eigenvalues appears (by increasing of α) are determined by $\alpha_n^2 + \beta^2 = k_n^2$, where $k_n^2 := ((2n + 1)\pi/4a)^2$ for some $n \in \mathbb{N}$.*

The eigenvalues $\lambda = k^2$ of $H^0_{\mathrm{I}(0)}(\alpha, \beta)$ are determined ($k = 0$ is admissible only if $\alpha = \beta = 0$) by the equation

$$(k^2 - \alpha^2 - \beta^2)\sin(2ka) - 2\beta k\cos(2ka) = 0. \tag{7.55}$$

The corresponding eigenfunctions read

$$\psi(x) = C\left(\cos(kx) + \frac{k\sin(ka) - (\mathrm{i}\alpha + \beta)\cos(ka)}{k\cos(ka) + (\mathrm{i}\alpha + \beta)\sin(ka)}\sin(kx)\right). \tag{7.56}$$

The eigenvalues of $H^m_{\mathrm{I}(0)}(\alpha, \beta)$ are obtained by adding m^2 to the eigenvalues of $H^0_{\mathrm{I}(0)}(\alpha, \beta)$.

Proof. We proceed in a similar way as in the alternative proof [37, Sect. 6.1] of the reality of the spectrum of $H^0_{\mathrm{I}(0)}(\alpha, 0)$. The original eigenvalue problem (7.53) with $m = 0$ can be transformed, using $\phi(x) := e^{\mathrm{i}\alpha x}\psi(x)$, into

$$\begin{cases} -\phi'' + 2\mathrm{i}\alpha\phi' + \alpha^2\phi = \lambda\phi & \text{in} \quad (-a, a), \\ \phi'(\pm a) \pm \beta\phi(\pm a) = 0. \end{cases} \tag{7.57}$$

We multiply the equation (7.57) by $\overline{\phi''}$ and integrate over $(-a, a)$. Next we multiply the complex conjugated version of the equation (7.57) by ϕ'' and again we integrate over $(-a, a)$. By subtracting the results and integrating by parts with use of the boundary conditions in (7.57), we obtain the identity

$$-\alpha\beta^2\left(|\phi(a)|^2 - |\phi(-a)|^2\right) = \Im\lambda\left(\|\psi'\|^2_{L^2(J_2)} + \beta(|\phi(a)|^2 + |\phi(-a)|^2)\right). \tag{7.58}$$

If we perform the same procedure, however, with multiplication by $\overline{\phi}$, after some integration by parts we receive the relation

$$\alpha\left(|\phi(a)|^2 - |\phi(-a)|^2\right) = \Im\lambda\,\|\phi\|^2_{L^2(J_2)}. \tag{7.59}$$

Combining (7.58) with (7.59) leads to the identity

$$0 = \Im\lambda\left(\|\phi'\|^2_{L^2(J_2)} + \beta(|\phi(a)|^2 + |\phi(-a)|^2) + \beta^2\|\phi\|^2_{L^2(J_2)}\right). \tag{7.60}$$

If β is positive, then the whole term in the brackets is strictly positive and thus imaginary part of λ must be zero. This proves the first item of the proposition.

If β is negative, then complex eigenvalues can appear. If we divide the equation (7.55) by k^2 and leave only $\sin(2ka)$ term on the left hand side, then it is clear that eigenvalues approach $(n\pi/2a)^2$ for k real and large enough. After simple algebraic manipulation (7.55) becomes

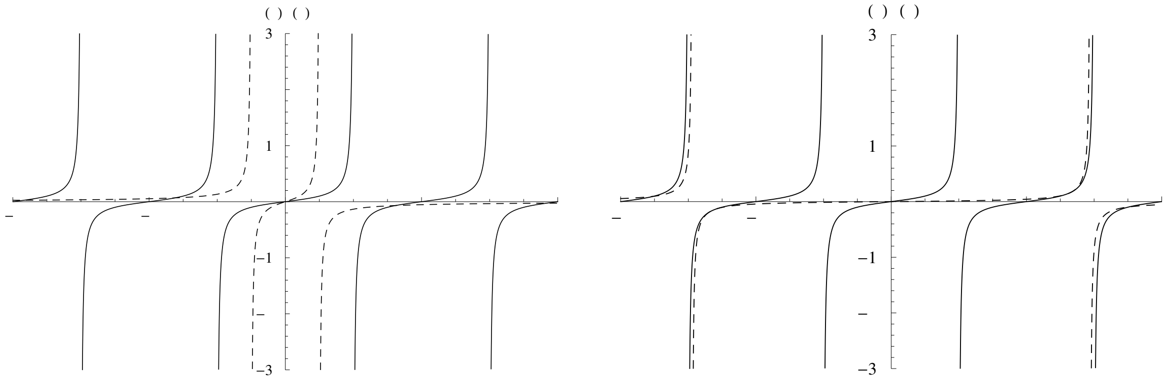
$$\tan(2ka) = \frac{2\beta k}{k^2 - \alpha^2 - \beta^2} \tag{7.61}$$

and the eigenvalues correspond to the intersections of the graphs of functions on left and right hand side of (7.61). We denote $l(k)$ the function on the left hand side, $r(k)$ the one on the right hand side, and $k_0 := \sqrt{\alpha^2+\beta^2}$. The behaviour of $r(k)$ for $k \in \mathbb{R}$ is summarized in Table 7.1. Graphs of functions $l(k)$

k	sign	asymptotics
$(-\infty,-k_0)$	$r(k)>0,\ r'(k)>0,\ r''(k)>0$	$\lim_{k\to -k_0-} r(k) = +\infty$ $\lim_{k\to-\infty} r(k) = 0$
$(-k_0,0)$	$r(k)<0,\ r'(k)>0,\ r''(k)<0$	$\lim_{k\to -k_0+} r(k) = -\infty$
$(0,k_0)$	$r(k)>0,\ r'(k)>0,\ r''(k)>0$	$\lim_{k\to k_0-} r(k) = +\infty$
(k_0,∞)	$r(k)<0,\ r'(k)>0,\ r''(k)<0$	$\lim_{k\to k_0-} r(k) = -\infty$ $\lim_{k\to\infty} r(k) = 0$

Table 7.1: The behaviour of $r(k)$.

and $r(k)$ are plotted in Figure 7.4. It is clear from the holomorphic dependence of eigenvalues on α,β (a



(a) $\alpha = 0$ (b) $\alpha = 3.1$

Figure 7.4: Graphs of $l(k)$ (full line) and $r(k)$ (dashed line), $a = \pi/4$, $\beta = -0.5$.

consequence of Theorem 7.2) that eigenvalues are close to $(n\pi/a)^2$, corresponding to zeros of $l(k) = \tan(2ka)$, except those in the neighbourhood of $\alpha^2+\beta^2$. Since $\alpha=\beta=0$ case corresponds to Neumann boundary conditions, for small α and β, all eigenvalues must be close to $(n\pi/2a)^2$. Hence, if we fix β and increase α, then two intersections of graphs of $l(k)$ and $r(k)$ are "lost" precisely at the point where $\alpha_n^2+\beta^2 = k_n^2$ for some $n\in\mathbb{N}$, *i.e.*, the asymptote of $r(k)$ corresponds to the asymptote of the tangent $l(k)$. This implies the creation of complex conjugate pair of eigenvalues. If we increase α more, two intersections appear again which means the annihilation of complex conjugate pair, *i.e.*, the restoration of two real eigenvalues. The two intersections are lost at the next critical value α_{n+1}. Very rough estimates give the location of restoration of real eigenvalues in the interval $(n\pi/2a, (2n+1)\pi/4a)$.

In view of the presented arguments, only one complex conjugated pair can appear in the spectrum for fixed α and β in the neighbourhood of $\alpha^2+\beta^2$, and the other eigenvalues approach $(n\pi/2a)^2$ as the distance from $\alpha^2+\beta^2$ increases. Moreover, for fixed β, the enlarging of α results into the shift of eigenvalues from almost Neumann ones $(n\pi/2a)^2, n\in\mathbb{N}$, to Dirichlet ones $((n+1)\pi/2a)^2, n\in\mathbb{N}$, for α large.

Finally, the equation for eigenvalues and eigenfunctions are found in a standard way. The general solution $A\cos(kx)+B\sin(kx)$ of $-\psi'' = k^2\psi$ is inserted into boundary conditions (7.53) and the condition for existence of non-trivial solutions A, B is the eigenvalue equation (7.55). □

Figures 7.5, 7.6 represent the α-dependence of the first four eigenvalues as obtained by a numerical analysis of (7.55). The numerical results confirm the above described behaviour. Let us remark that if β is positive, then the graph of $r(k)$ is reflected by the x-axis and the effect of loosing intersections is not possible, hence the spectrum remains real.

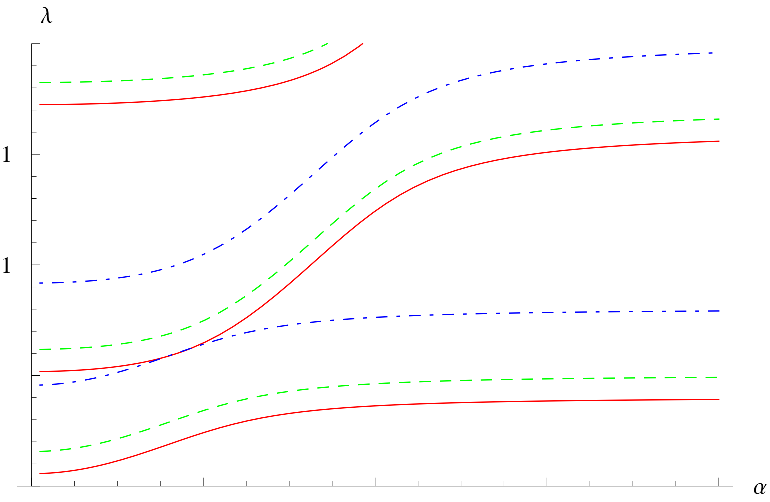


Figure 7.5: α-dependence of eigenvalues, zero curvature, $a = \pi/4$, $\beta = 0.5$. Red (full), green (dashed), and blue (dot-dashed) curves correspond to $m = 0, 1, 2$ respectively.

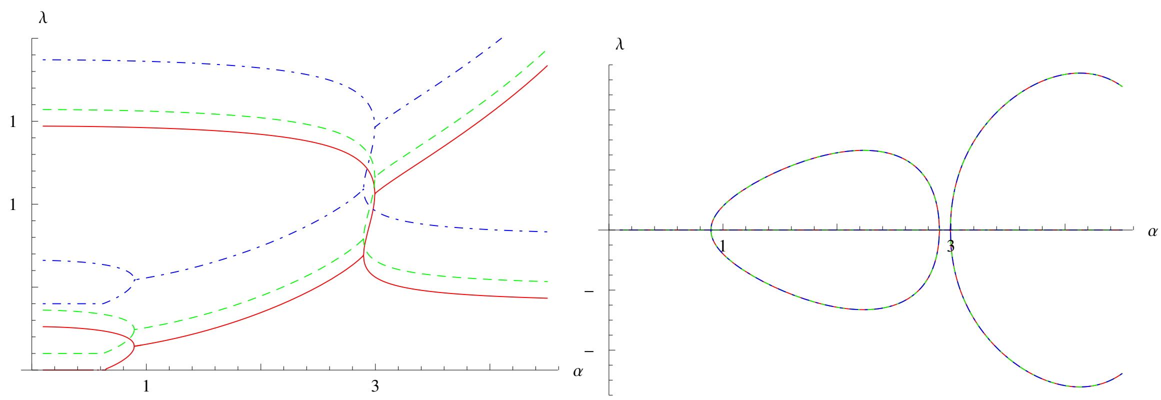


Figure 7.6: α-dependence of eigenvalues, zero curvature, $a = \pi/4$, $\beta = -0.5$. Red (full), green (dashed), and blue (dot-dashed) curves correspond to $m = 0, 1, 2$ respectively.

Positive curvature

The eigenvalue problem for the Hamiltonian $H^m_{\mathrm{I}(+1)}$ reads

$$\begin{cases} -\psi''(x) + \tan x\,\psi'(x) + \dfrac{m^2}{\cos^2 x}\psi(x) = k^2\psi(x) \quad \text{in} \quad (-a, a), \\ \psi'(\pm a) + \mathrm{i}\alpha\psi(\pm a) = 0. \end{cases} \tag{7.62}$$

Solutions of (7.62) can be written down in terms of associated Legendre functions $P^{(\mu)}_\nu, Q^{(\mu)}_\nu$:

$$\psi(x) = C_1\psi_1(x) + C_2\psi(x) \equiv C_1 P^{(m)}_\nu(\sin x) + C_2 Q^{(m)}_\nu(\sin x), \tag{7.63}$$

where

$$\nu := \frac{1}{2}\left(\sqrt{1+4\lambda} - 1\right), \tag{7.64}$$

$$C_2(\alpha\psi_2(-a) - \mathrm{i}\psi_2'(-a)) = C_1(-\alpha\psi_1(-a) + \mathrm{i}\psi_1'(-a)). \tag{7.65}$$

Inserting the general solution (7.63) into boundary conditions in (7.62) and consequent search for non-trivial constants C_1, C_2 yields the eigenvalue equation

$$\begin{vmatrix} \psi_1'(a) + \mathrm{i}\alpha\psi_1(a) & \psi_2'(a) + \mathrm{i}\alpha\psi_2(a) \\ \psi_1'(-a) + \mathrm{i}\alpha\psi_1(-a) & \psi_2'(a) + \mathrm{i}\alpha\psi_2(a) \end{vmatrix} = 0. \tag{7.66}$$

In order to analyse the spectrum in more details, we transform the Hamiltonian $H^m_{\mathrm{I}(+1)}$ into a unitarily equivalent operator of a more convenient form. The proof of the lemma is a straightforward calculation.

Lemma 7.6. *The unitary mapping* $U_{(+1)} : L^2(J_2, \mathrm{d}x) \to L^2(J_2, \mathrm{d}\nu_{(+1)})$

$$\left(U_{(+1)}\psi\right)(x) := (\cos x)^{-\frac{1}{2}}\,\psi(x) \tag{7.67}$$

transforms $H^m_{\mathrm{I}(+1)}(\alpha, 0)$ *to*

$$U^{-1}_{(+1)} H^m_{\mathrm{I}(+1)}(\alpha,0) U_{(+1)} = H^0_{\mathrm{I}(0)}(\alpha, \tfrac{1}{2}\tan a) + V^m_{(+1)}, \tag{7.68}$$

where

$$V^m_{(+1)}(x) := \frac{8m^2 - 3 - \cos 2x}{8\cos^2 x}. \tag{7.69}$$

Equipped with the equivalent form of the Hamiltonian, we prove the following result.

Proposition 7.5. *For every* $m \in \mathbb{Z}$ *there exists a real number* $\Lambda^m_{(+1)}$ *such that all eigenvalues* λ *with* $\Re\lambda \geq \Lambda^m_{(+1)}$ *are real and simple (*i.e. *the algebraic multiplicity being one). The eigenvalues with* $\Re\lambda < \Lambda^m_{(+1)}$ *can be complex, ordered in complex conjugated pairs.*

Eigenvalues are determined by equation (7.66) *and eigenfunctions can be written in the form* (7.63) *with* (7.65).

Proof. We follow standard arguments of perturbation theory (see *e.g.* [18] for spectral operators). Let us consider the transformed Hamiltonian (7.68) and forget about the potential for a moment, *i.e.*, we understand the potential $V^m_{(+1)}$ as a perturbation of $H^0_{\mathrm{I}(0)}(\alpha, \frac{1}{2}\tan a)$. Since $\tan a$ is positive under the assumption $a < \pi/2$, the reality of the spectrum is guaranteed by Proposition 7.4.1. The potential represents a bounded perturbation and it can shift eigenvalues only by $C\|V^m_{(+1)}\|$. Here the constant C comes from the estimate of the norm of the resolvent

$$\|R^0_{\mathrm{I}(0)}(\lambda)\| \leq \frac{C}{\Im\lambda}\,,$$

which is valid for $H^0_{\mathrm{I}(0)}(\alpha, \frac{1}{2}\tan a)$ due to the similarity to a normal operator (*cf* Theorem 7.2). The separation distance $|\lambda_{n+1} - \lambda_n|$ of eigenvalues (ordered with respect to the real part) of the unperturbed operator $H^0_{\mathrm{I}(0)}(\alpha, \frac{1}{2}\tan a)$ grows to infinity and two eigenvalues must collide at first to create a complex conjugate pair. Hence, the perturbed operator cannot have more than finitely many complex eigenvalues. Recall that due to $\mathcal{PT}$-symmetry (Corollary 7.2) the complex eigenvalues come in complex conjugated pairs. □

Remark 7.8. In other words, we detected the effects of positive curvature. It acts as the adding of real bounded potential $V^m_{(+1)}$ and real "β like" term in the boundary conditions to the zero curvature Hamiltonian $H^0_{\mathrm{I}(0)}$. The positive $\frac{1}{2}\tan a$ term is decisive for the behaviour of the spectrum, the bounded potential $V^m_{(+1)}$ can affect substantially only the lowest eigenvalues. Nonetheless, we conjecture that the spectrum remain real for every $m \in \mathbb{Z}$.

A numerical analysis of the equation (7.66) for $\lambda = k^2$ is presented in Figure 7.7. Obvious similarity with Figure 7.5 supports the perturbative results.

Negative curvature

The eigenvalue problem for the Hamiltonian $H^m_{\mathrm{I}(-1)}$ reads

$$\begin{cases} -\psi''(x) - \tanh x\,\psi'(x) + \dfrac{m^2}{\cosh^2 x}\psi(x) = k^2\psi(x) \quad \text{in} \quad (-a,a), \\ \psi'(\pm a) + \mathrm{i}\alpha\psi(\pm a) = 0. \end{cases} \tag{7.70}$$

The solutions of (7.70) can be again expressed via associated Legendre functions $P^{(\mu)}_\nu, Q^{(\mu)}_\nu$, but they have a little bit more complicated form then (7.63):

$$\psi(x) = C_1\psi_1(x) + C_2\psi(x) \equiv C_1\frac{P^{(\mu)}_\nu(\tanh x)}{\sqrt{\cosh x}} + C_2\frac{Q^{(\mu)}_\nu(\tanh x)}{\sqrt{\cosh x}}, \tag{7.71}$$

where

$$\mu := \mathrm{i}m - \frac{1}{2}, \quad \nu := \frac{1}{2}\sqrt{1-4\lambda}. \tag{7.72}$$

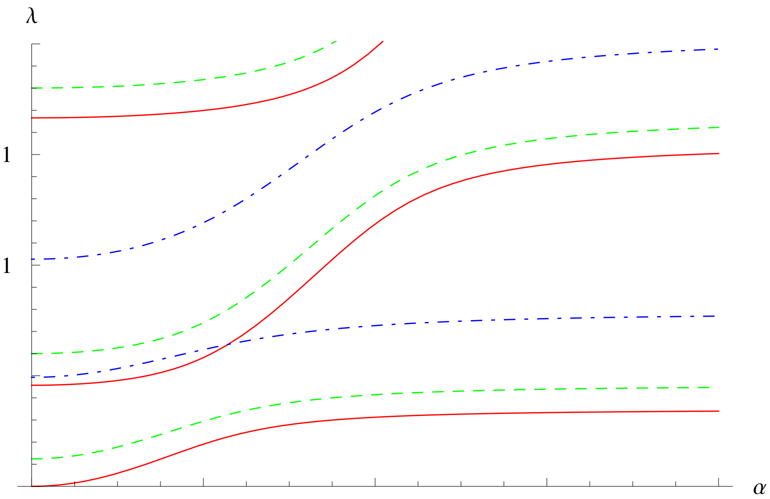


Figure 7.7: α-dependence of eigenvalues, positive curvature, $a = \pi/4$. Red (full), green (dashed), and blue (dot-dashed) curves correspond to $m = 0, 1, 2$ respectively.

Relations between C_1, C_2 can be obtained from equation (7.65), however, with ψ_1, ψ_2 corresponding to the negative curvature solutions (7.71); the same is true for the eigenvalue equation (7.66).

To explain the behaviour of the spectrum in a deeper way, we use the same strategy as in the positive curvature case. The eigenvalue problem (7.70) can be transformed by an analogous unitary transformation leading to a modified zero curvature eigenvalue problem.

Lemma 7.7. *The unitary mapping* $U_{(-1)} : L^2(J_2, \mathrm{d}x) \to L^2(J_2, \mathrm{d}\nu_{(-1)})$

$$\left(U_{(-1)}\psi\right)(x) := (\cosh x)^{-\frac{1}{2}}\,\psi(x) \tag{7.73}$$

transforms $H^m_{\mathrm{I}(-1)}(\alpha, 0)$ *to*

$$U^{-1}_{(-1)} H^m_{\mathrm{I}(-1)}(\alpha, 0) U_{(-1)} = H^0_{\mathrm{I}(0)}(\alpha, -\frac{1}{2}\tanh a) + V^m_{(-1)}, \tag{7.74}$$

where

$$V^m_{(-1)}(x) := \frac{8m^2 + 3 + \cosh 2x}{8\cosh^2 x}. \tag{7.75}$$

Proposition 7.6. *For every* $m \in \mathbb{Z}$ *there exists a real number* $\Lambda^m_{(-1)}$ *such that all eigenvalues* λ *with* $\Re\lambda \geq \Lambda^m_{(-1)}$ *are either real and simple (*i.e. *the algebraic multiplicity being one), or there is one complex conjugated pair of eigenvalues with real part located in the neighbourhood of* $\alpha^2 + \beta^2$*. The eigenvalues with* $\Re\lambda < \Lambda^m_{(-1)}$ *can be complex, ordered in complex conjugated pairs.*

Eigenvalues are determined by equation (7.66) *with* ψ_1, ψ_2 *from* (7.71)*. Eigenfunctions can be written in the form* (7.71) *with constants* C_1, C_2 *satisfying* (7.65) *with* ψ_1, ψ_2 *from* (7.71)*.*

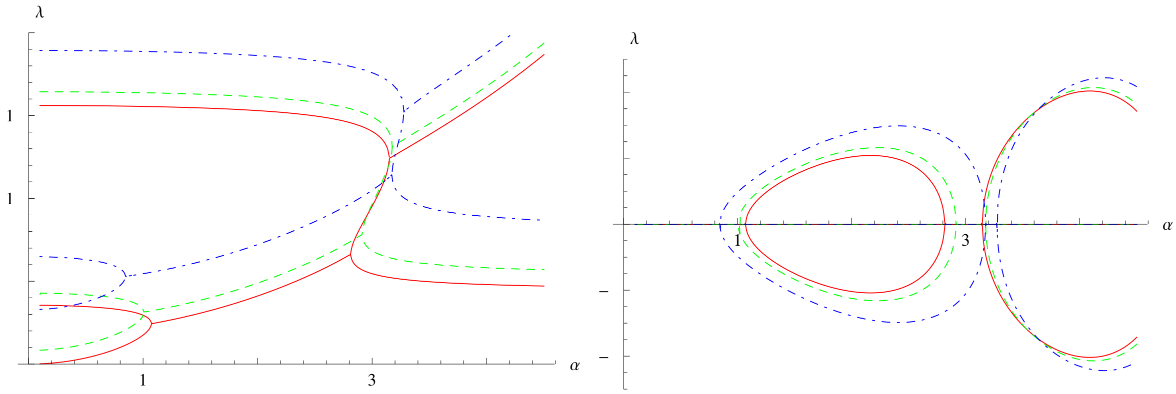
Proof. The proof is the same as in the positive curvature case, *cf* the proof of Proposition 7.5. The unperturbed Hamiltonian $H^0_{\mathrm{I}(0)}(\alpha, -\frac{1}{2}\tanh a)$ corresponds to the case analysed in Proposition 7.4.2. □

Remark 7.9. The curvature effect is now represented by the bounded real potential $V^m_{(-1)}$ and the extra negative term $-\frac{1}{2}\tanh a$ in the boundary conditions. The lowest eigenvalues (in absolute values) can be complex, nonetheless, we showed that the creation of a complex pair of eigenvalues is always followed by its annihilation, *i.e.* the restoration of real eigenvalues, when parameter α is increased.

A result of the numerical analysis of the eigenvalue problem is presented in Figure 7.8. The resemblance to zero curvature case with negative β in boundary conditions is obvious.

7.4.5 Connected boundary conditions

The connected boundary conditions are, by their nature, more complicated than the separated ones and moreover, they are given by three real parameters b, c, ϕ. Like for the separated boundary conditions, we can use the unitary transformations $U_{(\pm 1)}$ introduced in (7.67), (7.73) to transform the problems to the zero curvature



(a) Real part of λ (b) Imaginary part of λ

Figure 7.8: α-dependence of eigenvalues, negative curvature, $a = \pi/4$. Red (full), green (dashed), and blue (dot-dashed) curves correspond to $m = 0, 1, 2$ respectively. See animation, for an animated visualization of the α-dependence of the eigenvalues.

case, however, with modified boundary conditions and with additional bounded real potentials $V^m_{(\pm 1)}$ defined in (7.69), (7.75). The modification of boundary conditions is presented in appropriate subsections below.

The spectrum is not analytically described so far even for the zero curvature model and it is beyond the scope of this article to proceed with this analysis. The main aim of this section is to show the effect of curvature, *i.e.*, the transformation of curved models to the zero curvature case. Furthermore, we present some results of a numerical analysis for the 'lowest' eigenvalues: ϕ-dependence for selected values of b, c. It is important to note that, unlike in the separated case, we do not start with our parameters b, c, ϕ from a self-adjoint operator for $\phi = 0$, as it was the case for $\alpha = 0$ in the case of separated boundary conditions. We remark that the case $b = c = 0$, $\phi = \pm\pi/2$ corresponds to irregular boundary conditions and the spectrum of such operators is completely different from the cases presented here (*cf* [54]).

Zero curvature

We impose connected boundary conditions (7.19II) on the solutions of eigenvalue problem for $H^0_{\mathrm{II}(0)}(b, c, \phi)$ and we obtain the following equation for eigenvalues $\lambda = k^2$

$$-2k + 2k\cos(2ak)\sqrt{1+bc}\,\cos\phi + \left(bk^2 - c\right)\sin(2ak) = 0 \tag{7.76}$$

and eigenfunctions

$$\psi(x) = C_1\cos(kx) + C_2\sin(kx), \tag{7.77}$$

where the constants are further restricted by

$$C_2\left(\left(-1+\sqrt{1+bc}\,e^{\mathrm{i}\phi}\right)\cos(ak) + bk\sin(ak)\right) = C_1\left(\left(1+\sqrt{1+bc}\,e^{\mathrm{i}\phi}\right)\sin(ak) - bk\cos(ak)\right). \tag{7.78}$$

Proposition 7.7. *Eigenvalues* $\lambda = k^2$ *of* $H^0_{\mathrm{II}(0)}(b, c, \phi)$ *are determined by equation* (7.76)*, eigenfunctions read* (7.77) *with* (7.78)*.*

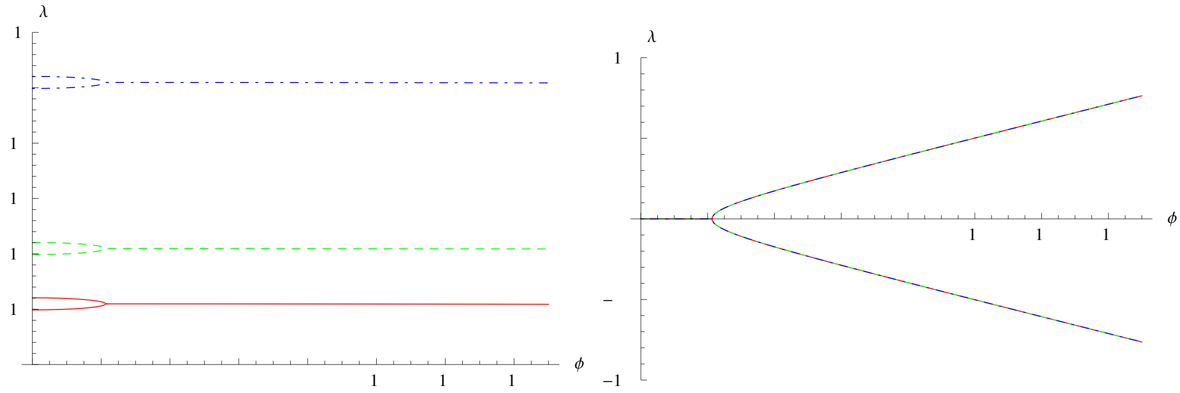
Eigenvalues for $m \neq 0$ *can be obtained by the shift* $\lambda \mapsto \lambda + m^2$ *while the corresponding eigenfunctions remain the same.*

Figure 7.9 illustrates the behaviour of eigenvalues for a certain choice of parameters.

Positive curvature

The solutions of the eigenvalue problem for $H^m_{\mathrm{II}(+1)}(b, c, \phi)$ with connected boundary conditions (7.19II) are the same as (7.63) except the constants C_1, C_2 now satisfy

$$C_2\left(\sqrt{1+bc}\,e^{\mathrm{i}\phi}\psi_2(-a) - \psi_2(a) + b\psi_2'(-a)\right) = C_1\left(\sqrt{1+bc}\,e^{\mathrm{i}\phi}\psi_1(-a) - \psi_1(a) + b\psi_1'(-a)\right). \tag{7.79}$$



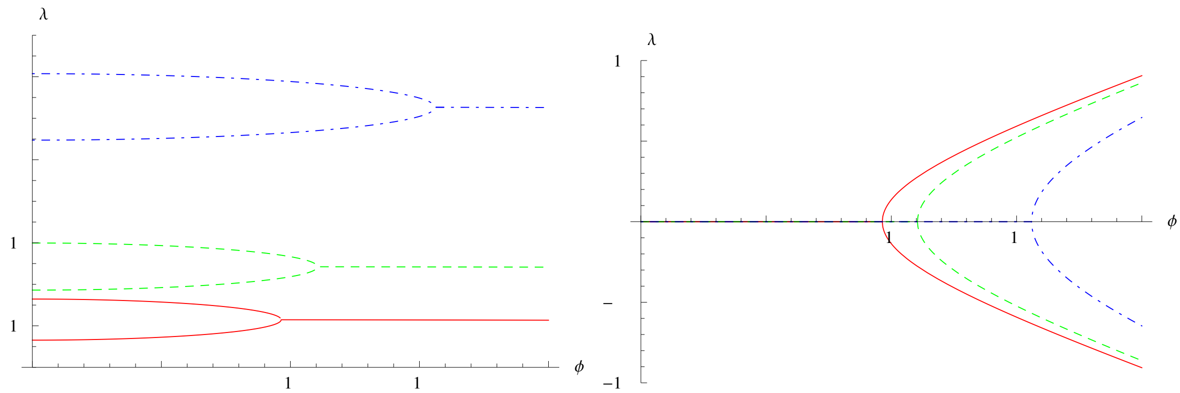
(a) Real part of λ (b) Imaginary part of λ

Figure 7.9: ϕ-dependence of eigenvalues, zero curvature, $a = \pi/4$, $b = c = 0.01$. Red (full), green (dashed), and blue (dot-dashed) curves correspond to $m = 0, 1, 2$ respectively.

The equation for eigenvalues reads

$$\begin{vmatrix} -\sqrt{1+bc}\,e^{\mathrm{i}\phi}\psi_1(-a) + \psi_1(a) - b\psi_1'(-a) & -\sqrt{1+bc}\,e^{\mathrm{i}\phi}\psi_2(-a) + \psi_2(a) - b\psi_2'(-a) \\ -c\psi_1(-a) - \sqrt{1+bc}\,e^{-\mathrm{i}\phi}\psi_1'(-a) + \psi_1'(a) & -c\psi_2(-a) - \sqrt{1+bc}\,e^{-\mathrm{i}\phi}\psi_2'(-a) + \psi_2'(a) \end{vmatrix} = 0. \tag{7.80}$$

Figure 7.10 illustrates the behaviour of eigenvalues for a certain choice of the parameters.



(a) Real part of λ (b) Imaginary part of λ

Figure 7.10: ϕ-dependence of eigenvalues, positive curvature, $a = \pi/4$, $b = c = 0.01$. Red (full), green (dashed), and blue (dot-dashed) curves correspond to $m = 0, 1, 2$ respectively.

We employ the unitary transformation $U_{(+1)}$ introduced in Lemma 7.6 to map $H^m_{\mathrm{II}(+1)}(b,c,\phi)$ to a zero curvature Hamiltonian.

Proposition 7.8. *The unitary mapping $U_{(+1)}$ defined in (7.67) transforms the Hamiltonian $H^m_{\mathrm{II}(+1)}(b,c,\phi)$ to*

$$U^{-1}_{(+1)} H^m_{\mathrm{II}(+1)}(b,c,\phi) U_{(+1)} = \hat{H}^0_{\mathrm{II}(0)} + V^m_{(+1)}, \tag{7.81}$$

where $V^m_{(+1)}$ is defined in (7.69) and $\hat{H}^0_{\mathrm{II}(0)} := -\dfrac{\mathrm{d}^2}{\mathrm{d}x^2}$ with the domain consisting of $\psi \in W^{2,2}(J_2)$ satisfying

$$\begin{aligned} \Psi(a) &= B_{(+1)}\Psi(-a), \quad \text{with } \Psi(x) := \begin{pmatrix} \psi(x) \\ \psi'(x) \end{pmatrix} \text{ and} \qquad (7.82) \\ B_{(+1)} &:= \begin{pmatrix} \sqrt{1+bc)}\,e^{\mathrm{i}\phi} - \frac{1}{2}b\tan a & b \\ c - \sqrt{1+bc}\tan a\cos\phi + \frac{1}{4}b\tan^2 a & \sqrt{1+bc}\,e^{-\mathrm{i}\phi} - \frac{1}{2}b\tan a \end{pmatrix}. \end{aligned}$$

Eigenvalues $\lambda = k^2$ of $H^m_{\mathrm{II}(+1)}(b,c,\phi)$ are determined by equation (7.80), eigenfunctions read (7.63) with constants C_1, C_2 given by (7.79).

Remark 7.10. The boundary conditions (7.82) are $\mathcal{PT}$-symmetric, but they are no more $\mathcal{P}$-pseudo-Hermitian. This result shows that although we reduced the problem to the zero curvature case (in the sense of previous sections), the investigation of spectrum must be done with more general boundary conditions than $\mathcal{PT}$-symmetric and $\mathcal{P}$-pseudo-Hermitian at the same time.

Negative curvature

The solutions of the eigenvalue problem for $H^m_{\mathrm{II}(-1)}(b,c,\phi)$ with connected boundary conditions (7.19II) are the same as in the separated conditions case (7.71), but the relation between constants C_1, C_2 is given by (7.79) with ψ_1, ψ_2 corresponding to the negative curvature solutions (7.71); the same is also valid for the eigenvalue equation (7.80).

Figure 7.11 illustrates the behaviour of eigenvalues for a certain choice of parameters.

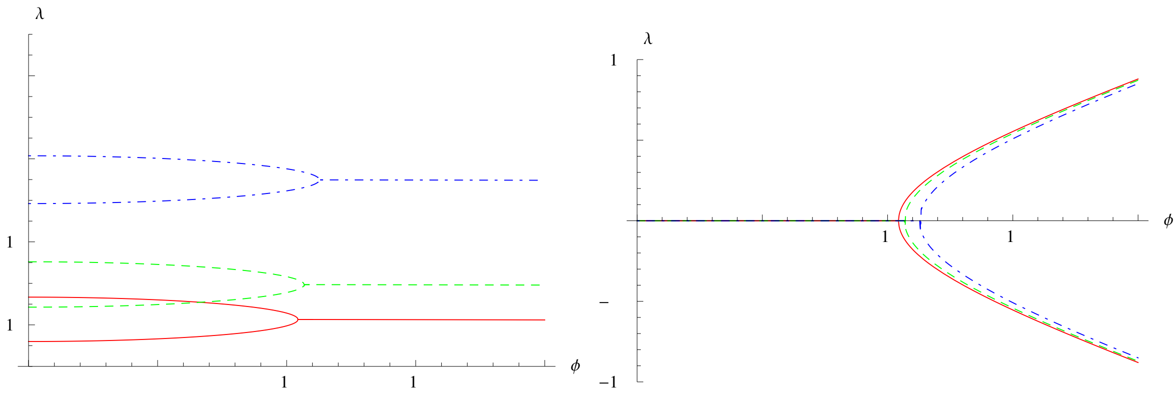


Figure 7.11: ϕ-dependence of eigenvalues, negative curvature, $a = \pi/4$, $b = c = 0.01$. Red (full), green (dashed), and blue (dot-dashed) curves correspond to $m = 0, 1, 2$ respectively.

Proposition 7.9. *The unitary mapping $U_{(-1)}$ defined in* (7.73) *transforms the Hamiltonian $H^m_{\mathrm{II}(-1)}(b,c,\phi)$ to*

$$U^{-1}_{(-1)} H^m_{\mathrm{II}(-1)}(b,c,\phi) U_{(-1)} = \tilde{H}^0_{\mathrm{II}(0)} + V^m_{(-1)}, \tag{7.83}$$

where $V^m_{(-1)}(x)$ is defined in (7.75) *and $\tilde{H}^0_{\mathrm{II}(0)} := -\dfrac{\mathrm{d}^2}{\mathrm{d}x^2}$ with the domain consisting of $\psi \in W^{2,2}(J_2)$ satisfying*

$$\begin{aligned} \Psi(a) &= B_{(-1)}\Psi(-a), \quad \text{with } \Psi(x) := \begin{pmatrix} \psi(x) \\ \psi'(x) \end{pmatrix} \text{ and} \\ B_{(-1)} &:= \begin{pmatrix} \sqrt{1+bc)}\, e^{\mathrm{i}\phi} + \frac{1}{2} b \tanh a & b \\ c + \sqrt{1+bc} \tanh a \cos\phi + \frac{1}{4} b \tanh^2 a & \sqrt{1+bc}\, e^{-\mathrm{i}\phi} + \frac{1}{2} b \tanh a \end{pmatrix}. \end{aligned} \tag{7.84}$$

Eigenvalues $\lambda = k^2$ of $H^m_{\mathrm{II}(-1)}(b,c,\phi)$ are determined by equation (7.80) *with ψ_1, ψ_2 from* (7.71). *The eigenfunctions read* (7.71), *where constants C_1, C_2 are given by* (7.79) *with ψ_1, ψ_2 from* (7.71).

Remark 7.11. The boundary conditions (7.84) are $\mathcal{PT}$-symmetric, however not $\mathcal{P}$-pseudo-Hermitian, as for the positive curvature case. Thus again, it is necessary to investigate more general boundary conditions in zero curvature eigenvalue problem.

7.5 Concluding remarks

The goal of this paper was to introduce a new class of $\mathcal{PT}$-symmetric Hamiltonians defined in curved manifolds and describe the effects of curvature on the spectrum. Although we were able to find these effects for both separated and connected boundary conditions, the absence of results on reality of the spectrum for the latter (even in the case of zero curvature) did not allow us to present the conclusions in an entirely descriptive and explicit way. Let us therefore summarize the main features of the model for the separated Robin type boundary conditions (7.3) only.

curvature	spectrum	eigenvalues
zero	$\mathbb{R}$	only some α-dependent, crossings
positive	$\mathbb{R}$	all α-dependent, no crossings
negative	$\mathbb{C}$	all α-dependent, crossings, creation and annihilation of complex pairs

Table 7.2: A heuristic summary of our analytical and numerical analysis.

In Table 7.2 we schematically (and very roughly) describe qualitative properties of the spectrum we observed in the constant-curvature cases. The entry describing the positive curvature case includes our conjecture (supported by numerical analysis) that all eigenvalues are real.

One of the most instructive results in the paper are probably Lemmata 7.6 and 7.7, which enable one to understand the effect of curvature in terms of an additional effective potential and boundary-coupling interaction. For the s-wave modes (*i.e.* $m = 0$ in the decomposition (7.43)) and infinitesimally thin strips (*i.e.* $a \ll l$), it follows from the lemmata that the positive and negative curvature acts as an attractive and repulsive interaction, respectively. This is in agreement with a spectral analysis of similar models in the self-adjoint case of Dirichlet boundary conditions [34, 35]. However, the additional boundary interaction is not negligible for positive widths a, and its effect is actually completely opposite (*cf* Remarks 7.8, 7.9): the positive and negative curvature gives rise to an attractive and repulsive Robin-type boundary condition, respectively. The interplay between these two effects is further complicated by the presence of the repulsive centrifugal term for $|m| \geq 1$, and the numerical analysis confirms that the overall picture of the spectrum can be quite complex.

It follows from previous comments and remarks that there remain several open problems, *e.g.* the proof of the reality of all eigenvalues in the positive curvature model. Nonetheless, we would like to mention also some other interesting directions of potential future research: the spectral effect of curvature in non-constant curvature and non-constant boundary-coupling functions setting, the existence of Riesz basis for such setting or models defined on unbounded domains (waveguides) in curved spaces. The last case can be viewed as a natural continuation of [10] where a planar $\mathcal{PT}$-symmetric waveguide was studied.

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Chapter 8

The Pauli equation with complex boundary conditions

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The Pauli equation with complex boundary conditions

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Abstract. We consider one-dimensional Pauli Hamiltonians in a bounded interval with possibly non-self-adjoint Robin-type boundary conditions. We study the influence of the spin-magnetic interaction on the interplay between the type of boundary conditions and the spectrum. A special attention is paid to $\mathcal{PT}$-symmetric boundary conditions with the physical choice of the time-reversal operator $\mathcal{T}$.

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Keywords: Pauli equation, spin-magnetic interaction, Robin boundary conditions, non-self-adjointness, non-Hermitian quantum mechanics, $\mathcal{PT}$-symmetry, time-reversal operator

8.1 Introduction

In recent years there has been a growing interest in non-Hermitian "extensions" of quantum mechanics, usually associated with the names of *$\mathcal{PT}$-symmetry*, *pseudo-Hermiticity*, *quasi-Hermiticity* or *crypto-Hermiticity* (we respectively refer to [4, 29, 31, 39] where the first two works are recent surveys with many references). The quotation marks are used here because the extended theories are physically relevant only if the operators in question are *similar to self-adjoint* operators, which in turn puts the concept back to the conventional quantum mechanics.

However, the freedom related to the existence of the similarity transformation can be highly useful in applications, since a complicated non-local self-adjoint operator can be represented by a (possibly non-self-adjoint) differential operator (see [23] for one-dimensional examples), and the spectral theory for the latter is much more developed. Moreover, it is necessary that the non-Hermitian operators possess *real spectra*, which can be often ensured (at least in some perturbative regimes [9, 27]) by the simple criterion of $\mathcal{PT}$-symmetry.

The goal of the present paper is to examine the role of *spin* in the above theories. We consider the simplest non-trivial situation of an electron (spin $\frac{1}{2}$, mass m, charge $-e<0$) interacting exclusively with an external homogeneous magnetic field $\vec{B}\in\mathbb{R}^3$. Choosing the Poincaré gauge in which the magnetic vector potential coincides with $\frac{1}{2}\vec{B}\times\vec{x}$, this system is governed by the *Pauli equation*

$$i\hbar\frac{\partial\Psi}{\partial t}=-\frac{\hbar^2}{2m}\,\Delta\Psi+\frac{\mu}{\hbar}\,\vec{B}\cdot\vec{L}\,\Psi+\frac{e^2}{8m}\,(\vec{B}\times\vec{x})^2\Psi+\mu\,\vec{B}\cdot\vec{\sigma}\,\Psi=:H\Psi \tag{8.1}$$

in the space-time variables $(\vec{x},t)$, where $\hbar$ is the reduced Planck constant, $\mu:=\hbar e/(2m)$ is the Bohr magneton (for simplicity), $\vec{L}$ is the angular-momentum operator and $\vec{\sigma}$ is a three-component vector formed by the Pauli matrices. The spinorial wavefunction Ψ can be represented as an element of $L^2(\mathbb{R}^3)\otimes\mathbb{C}^2$ and the operators appearing in (8.1) are assumed to appropriately act in this Hilbert space.

The Hamiltonian H (equipped with a suitable domain) is Hermitian when considered in the full Hilbert space $L^2(\mathbb{R}^3)\otimes\mathbb{C}^2$. Moreover, the Pauli equation (8.1) is invariant under a simultaneous reversal of the space and time variables (*cf* the discussion in Section 8.5). Relying on general definitions for the Dirac field (see, *e.g.*, [5, §26]) and the fact that the Pauli equation can be obtained from the Dirac equation in a non-relativistic limit, the discrete symmetries can be represented by means of the *parity* $\mathcal{P}$ and the *time-reversal operator* $\mathcal{T}$ (uniquely determined up to a phase factor).

Our way how to "complexify" (8.1) is to restrict the space variables to a subset $\Omega\subset\mathbb{R}^3$ and impose *complex boundary conditions* of the Robin type

$$\frac{\partial\Psi}{\partial n}+A\Psi=0 \qquad \text{on} \qquad \partial\Omega\,, \tag{8.2}$$

where n is the outward pointing normal unit to $\partial\Omega$ and A is a two-by-two complex-valued matrix. If Ω is invariant with respect to the spatial inversion $\mathcal{P}$, it is possible to choose A in such a way that the $\mathcal{PT}$-symmetry of (8.1) remains valid for the (possibly non-Hermitian) operator H on $L^2(\Omega) \otimes \mathbb{C}^2$, subject to the boundary conditions (8.2).

In this paper we study the interplay between the form of the matrix A and the spectrum of H. In particular, we are interested in the existence of real eigenvalues in the $\mathcal{PT}$-symmetric situation.

We are not aware of previous works on Pauli equation in the non-Hermitian extensions of quantum mechanics. However, there exist results on spinorial systems in the context of $\mathcal{PT}$-symmetric coupled-channels models [36, 37, 38] and the Dirac equation in the framework of Krein spaces [1, 24].

One of the reasons for considering the spinorial model in this paper is the fact that the time-reversal operator $\mathcal{T}$ *differs from the complex conjugation*, the latter being the time-reversal operator for the scalar (*i.e.* spinless) Schrödinger equation, widely studied in the $\mathcal{PT}$-symmetric quantum theory. In fact, for fermionic systems (*i.e.* half-integer non-zero spin), one has

$$\mathcal{T}^2 = -1\,. \tag{8.3}$$

This has been remarked previously in the context of pseudo-Hermitian operators in [32, 6]. A generalized concept of $\mathcal{PT}$-symmetry as regards the operator $\mathcal{P}$ is suggested in [35].

The present model can be regarded as an extension of the one-dimensional scalar Hamiltonians with complex Robin boundary conditions studied in [21, 20, 23] to the spinorial case. We refer to [22, 15] for the discussion of relevance of (possibly non-Hermitian) Robin boundary conditions in physics and, in particular, to Section 8.3 for a simple scattering-type interpretation in the present setting.

This paper is organized as follows. In the following section we specify our model in terms of a one-dimensional Hamiltonian coming from (8.1). A physical relevance of the boundary conditions (8.2) is suggested in Section 8.3. Section 8.4 is devoted to a rigorous definition of our Hamiltonian as a closed operator associated with a sectorial sesquilinear form. In Section 8.5 we discuss the physical choice of the operator $\mathcal{PT}$ and establish conditions on the boundary matrix A which guarantee various symmetry properties of the Hamiltonian. Section 8.6 is devoted to a spectral analysis supported by numerics; on several $\mathcal{PT}$-symmetric examples we discuss the dependence of the spectrum on parameters characterizing the matrix A. The paper is concluded by Section 8.7 in which we mention some open problems.

8.2 Our model

We begin specifying our model represented by the Pauli equation (8.1).

We choose the coordinate system in $\mathbb{R}^3$ in such a way that the third coordinate axis is parallel with the homogeneous magnetic field $\vec{B}$, *i.e.* $\vec{B} = (0,0,B)$ where $B \in \mathbb{R}$. Then the orbital interaction $\vec{B}\cdot\vec{L}$ and the diamagnetic term $(\vec{B}\times\vec{x})^2$ represent differential operators in the first two space variables only. On the other hand, the spinorial interaction $\vec{B}\cdot\vec{\sigma}$ acts in the third space variable only (through the Pauli matrix $\sigma_3 = \mathrm{diag}(1,-1)$).

We set

$$\Omega := \mathbb{R}^2 \times (-a, a)\,, \tag{8.4}$$

with some positive number a. Assuming that the matrix A in (8.2) is constant on each of the connected components of $\partial\Omega$, the spectral problem for the Hamiltonian H therefore splits into two separate problems: a two-dimensional Landau-level problem in the first two variables and a one-dimensional problem in the third variable which we will study in sequel. Up to a constant factor representing the energy of the given Landau level, the corresponding one-dimensional operators have the form

$$H_b = \begin{pmatrix} -\dfrac{\mathrm{d}^2}{\mathrm{d}x^2} + b & 0 \\ 0 & -\dfrac{\mathrm{d}^2}{\mathrm{d}x^2} - b \end{pmatrix} \qquad \text{on} \qquad \mathcal{H} := L^2\big((-a,a);\mathbb{C}^2\big)\,, \tag{8.5}$$

subject to the boundary conditions

$$\Psi'(\pm a) + A^{\pm}\Psi(\pm a) = 0\,. \tag{8.6}$$

Here we have put $\hbar^2/(2m) = 1$ and $b := \mu B$, $A^{\pm} \in \mathbb{C}^{2\times 2}$, and the third space variable is (with an abuse of notation) denoted by x.

In view of the choice of physical constants made above, the only distinguished length in our problem is the half-width a, and therefore the results must be scaled appropriately with respect to this length. In particular, the parameter b (characterizing the strength of the magnetic field) and eigenvalues of H_b (corresponding to quantum energies) become dimensionless when multiplied by a^2. The same can be done for the entries of $A^{\pm}$ when multiplied by a. Consequently, all parameters can be thought as dimensionless in the sequel.

As usual, the Hilbert space $\mathcal{H}$ is identified with $L^2((-a,a)) \otimes \mathbb{C}^2$ and its elements are represented by the two-component spinors

$$\Psi = \begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix},$$

where $\psi_\pm \in L^2((-a,a))$ (the $\pm$ notation should not be confused with the superscripts of the matrices $A^{\pm}$ referring to the endpoints of $(-a,a)$). The inner product in $\mathcal{H}$ is defined by

$$(\Phi, \Psi) := \int_{-a}^{a} \overline{\Phi}^T(x)\, \Psi(x)\, \mathrm{d}x\,,$$

where the upper index T denotes transposition. The corresponding norm is denoted by $\|\cdot\|$. The Euclidean norm of the spinor Ψ as a vector in $\mathbb{C}^2$ is denoted by $|\Psi| := \sqrt{|\psi_+|^2 + |\psi_-|^2}$ and we use the same notation for the corresponding operator (matrix) norm $|A| := \max\left\{|A\Psi| \,\middle|\, \Psi \in \mathbb{C}^2,\, |\Psi| = 1\right\}$ for $A \in \mathbb{C}^{2\times 2}$.

8.3 Scattering motivation

Before giving a rigorous definition of our Hamiltonian formally introduced (8.5)–(8.6), let us first justify the physical relevance of the boundary conditions (8.6). Our method is based on a generalization of an idea originally suggested in [15].

Consider a generalized eigenvalue problem for the Hamiltonian of the form (8.5) on the whole space $\mathbb{R}$ locally perturbed by an electric field:

$$\begin{pmatrix} -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + b + V(x) & 0 \\ 0 & -\frac{\mathrm{d}^2}{\mathrm{d}x^2} - b + V(x) \end{pmatrix} \begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix} = \lambda \begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix}. \tag{8.7}$$

Here $x \in \mathbb{R}$, $\lambda \in \mathbb{R}$ and V is the electric potential that is assumed to be compactly supported in $(-a,a)$. Solutions Ψ with $\lambda < -|b|$ are bound states (associated with discrete eigenvalues), while those with $\lambda \geq -|b|$ correspond to scattering states (associated with the essential spectrum).

Outside the support of V the problem (8.7) admits explicit solutions in terms of exponential functions. Let us look for special scattering solutions satisfying

$$\Psi(x) = \begin{pmatrix} e^{\mathrm{i}\sqrt{\lambda-b}\,x} \\ e^{\mathrm{i}\sqrt{\lambda+b}\,x} \end{pmatrix} \qquad \text{for} \qquad |x| \geq a\,. \tag{8.8}$$

Then the (physical) problem (8.7) on the whole real axis can be solved by considering an (effective) boundary value problem in $(-a,a)$. The latter is simply obtained by considering (8.7) in $(-a,a)$ and requiring that the solutions match at $\pm a$ smoothly with the asymptotic solutions (8.8). This leads to the boundary conditions (8.6) with an *energy-dependent* matrix

$$A_\lambda^{\pm} = \begin{pmatrix} -\mathrm{i}\sqrt{\lambda - b} & 0 \\ 0 & -\mathrm{i}\sqrt{\lambda + b} \end{pmatrix}. \tag{8.9}$$

Note that (8.7) for $x \in (-a,a)$, subject to (8.6) with (8.9) at $\pm a$, does not represent a standard spectral problem, it is rather an operator-pencil problem (because of the dependence of $A_\lambda^{\pm}$ on the spectral parameter λ). It is non-linear in its nature. However, it can be solved by first considering a genuine (linear) spectral problem, namely (8.7) for $x \in (-a,a)$, subject to (8.6) with $A_\alpha^{\pm}$ at $\pm a$, with α being treated as a real parameter. This leads to a discrete set of eigencurves $\alpha \mapsto \lambda_n(\alpha)$, $n \in \mathbb{N}$. Then the "eigenvalues" of the true, energy-dependent problem are determined as those points $\lambda_n(\alpha_*)$ satisfying the (non-linear) algebraic equations

$$\lambda_n(\alpha_*) = \alpha_*\,. \tag{8.10}$$

The elements of the set $\{\lambda_n(\alpha_*)\}_{n\in\mathbb{N}}$ are called *perfect-transmission energies* (PTEs) in [15], since their physical meaning is that they determine energies for which there is no reflection for the initial scattering problem (8.7) in $\mathbb{R}$. It is interesting that (8.10) admits the real PTEs solutions, since these are obtained via solving a highly non-self-adjoint spectral problem. This feature is related to the fact that the choice $A_\alpha^{\pm}$ ensures that the boundary conditions are $\mathcal{PT}$-symmetric (although not $\mathcal{PT}$-symmetric in the context of the present paper where we do not allow the presence of λ and b in the boundary conditions, see below). A physical interpretation of the possible complexification of the spectra of the auxiliar $\mathcal{PT}$-symmetric spectral problem is also proposed in [15].

It is also interesting to note that switching on the static magnetic field (*i.e.* making $b \neq 0$) will typically lead to a splitting of the doubly degenerate eigencurves corresponding to the auxiliar non-self-adjoint spectral problem for $b = 0$ (*cf* Figure 8.2). Consequently, to each of the PTE in the scalar case without the magnetic field there correspond two PTEs in our spinorial model. The analogy with the *Zeeman effect* should not be surprising.

The matrix (8.9) is complex and non-Hermitian, which is typical for effective models of scattering solutions of (8.7). On the other hand, real-valued Hermitian matrices are obtained when looking for bound states. In this paper, we proceed in a full generality by allowing *arbitrary* matrices $A^{\pm}$ in (8.6). However, it is important to stress that we regard the matrices as parameters entering the spectral system; the dependence of $A^{\pm}$ on the spectral parameter λ is not allowed and the dependence on the field b is allowed only if b is treated as a parameter (no change under the action of $\mathcal{T}$, *cf* Section 8.5).

To end up this motivation section, let us note that alternative proposals for the connection between non-Hermitian $\mathcal{PT}$-symmetric operators and physics have been suggested recently in the context of scattering in [16, 28, 34, 17].

8.4 The Pauli Hamiltonian

We now turn to a rigorous definition of the Hamiltonian formally introduced by (8.5)–(8.6). In other words, since we are interested in spectral properties, we need a closed realization of the operator H_b.

The easiest way is to define the Hamiltonian as the Friedrichs extension of the operator (8.5) initially considered on uniformly smooth spinors satisfying (8.6). On such a restricted domain, an integration by parts easily leads to the associated sesquilinear form h_b as a sum of three terms

$$h_b(\Phi,\Psi) = q_1(\Phi,\Psi) + b\, q_2(\Phi,\Psi) + q_3(\Phi,\Psi)\,, \tag{8.11}$$

where

$$\begin{aligned} q_1(\Phi,\Psi) &:= (\Phi',\Psi')\,,\\ q_2(\Phi,\Psi) &:= (\Phi,\sigma_3\Psi)\,,\\ q_3(\Phi,\Psi) &:= \overline{\Phi}^T(a)\, A^+\, \Psi(a) - \overline{\Phi}^T(-a)\, A^-\, \Psi(-a)\,. \end{aligned} \tag{8.12}$$

The form h_b is well defined on a larger, Sobolev-type space

$$\mathsf{D}(h_b) := H^1\big((-a,a);\mathbb{C}^2\big)\,. \tag{8.13}$$

It is obvious for q_1 and q_2, while the boundary term q_3 can be shown bounded on $\mathsf{D}(h_b)$ by means of the Sobolev embedding $H^1((-a,a)) \hookrightarrow C^0([-a,a])$.

Our aim is to show that h_b is a closed sectorial form. It is clear for q_1 defined on (8.13), since q_1 is associated with the Neumann Laplacian (*cf* [10, Sec. 7]), and as such it is a densely defined, closed, symmetric, non-negative form. The term q_2 represents just a bounded perturbation; indeed, $|q_2[\Psi]| \leq \|\Psi\|^2$ for every $\Psi \in \mathcal{H}$. While this is no longer true for q_3, a suitable quantification of the Sobolev embedding can be used to ensure that q_3 still represents a small perturbation in the following sense.

Lemma 8.1. *For every $\Psi \in \mathsf{D}(h_b)$ and $\varepsilon \in (0,1)$,*

$$\big|q_3[\Psi]\big| \leq \varepsilon\,\big(|A^+|+|A^-|\big)\,\|\Psi'\|^2 + \left(\frac{|A^+|+|A^-|}{2a} + \frac{|A^+|+|A^-|}{\varepsilon}\right)\|\Psi\|^2\,.$$

Consequently, the form $q_2 + q_3$ is relatively bounded with respect to q_1 and the relative bound can be made arbitrarily small.

Proof. The claim is based on the estimates

$$|\Psi(\pm a)|^2 \leq 2\,\|\Psi'\|\|\Psi\| + \frac{1}{2a}\,\|\Psi\|^2 \leq \varepsilon\,\|\Psi'\|^2 + \left(\frac{1}{2a}+\frac{1}{\varepsilon}\right)\|\Psi\|^2 \tag{8.14}$$

valid for any $\Psi \in \mathsf{D}(h_b)$. Here the first inequality can be established quite easily by the fundamental theorem of calculus and the Schwarz inequality. ☐

Consequently, the perturbation result [18, Thm.VI.1.33] can be used to show that h_b is indeed sectorial and closed. According to the first representation theorem [18, Thm.VI.2.1], there exists a unique m-sectorial operator H_b in $\mathcal{H}$ such that $h_b(\Phi,\Psi) = (\Phi, H_b\Psi)$ for all $\Phi \in \mathsf{D}(h_b)$ and $\Psi \in \mathsf{D}(H_b) \subset \mathsf{D}(h_b)$. Following the arguments [18, Ex. VI.2.16], it is easy to check that H_b indeed acts as (8.5)–(8.6); more precisely,

$$\begin{aligned} H_b\Psi &= \begin{pmatrix} -\psi_+'' + b\psi_+ \\ -\psi_-'' - b\psi_- \end{pmatrix}, \\ \mathsf{D}(H_b) &= \Big\{\Psi \in H^2\big((-a,a);\mathbb{C}^2\big) \ \big|\ \Psi'(\pm a) + A^\pm \Psi(\pm a) = 0\Big\}. \end{aligned} \tag{8.15}$$

Proposition 8.1. *H_b defined by (8.15) is an m-sectorial operator on $\mathcal{H}$. The adjoint of H_b is given by*

$$\begin{aligned} H_b^*\Psi &= \begin{pmatrix} -\psi_+'' + b\psi_+ \\ -\psi_-'' - b\psi_- \end{pmatrix}, \\ \mathsf{D}(H_b^*) &= \Big\{\Psi \in H^2\big((-a,a);\mathbb{C}^2\big) \ \big|\ \Psi'(\pm a) + (A^\pm)^* \,\Psi(\pm a) = 0\Big\}, \end{aligned} \tag{8.16}$$

where $A^* = \overline{A^T}$.

Proof. It remains to notice (*cf* [18, Thm. VI.2.5]) that the adjoint operator is determined as the m-sectorial operator associated with the adjoint form h_b^* defined by $h_b^*(\Phi,\Psi) := \overline{h_b(\Psi,\Phi)}$, $\mathsf{D}(h_b^*) := \mathsf{D}(h_b)$. □

Note that the choice $A^\pm = 0$ gives rise to the (self-adjoint) Pauli Hamiltonian, subject to Neumann boundary conditions, that we denote by H_b^N. (At the same time, the choice $A^\pm = \infty$ formally corresponds to Dirichlet boundary conditions.)

8.5 Symmetry properties

It is well known that the Pauli equation (8.1) (in the whole space $\mathbb{R}^3$) is invariant under the simultaneous space inversion and time reversal (*i.e.* $\vec{x} \mapsto -\vec{x}$ and $t \mapsto -t$, respectively). This can be easily established if one realizes that the time reversal leads to a change of orientation of the magnetic field (*i.e.* $\vec{B} \mapsto -\vec{B}$), while the orientation is unchanged by the space inversion. These properties can be deduced from Maxwell's equations to which the equation (8.1) is implicitly coupled (*cf* [26, §17]).

One is tempted to mathematically formalize the space-time reversal invariance in terms of a symmetry property of the Hamiltonian H. Given a unitary or antiunitary operator $\mathcal{C}$, we say that a linear operator H in a Hilbert space is $\mathcal{C}$-*symmetric* if

$$[H,\mathcal{C}] = 0\,. \tag{8.17}$$

Here the commutator relation should be interpreted as an operator identity on the domain of H, *i.e.* $\mathcal{C}H \subset H\mathcal{C}$. However, in this framework the Hamiltonian H appearing (8.1) is not $\mathcal{PT}$-symmetric, just because there is no way how ensure the change of sign $\vec{B}$ under the action of $\mathcal{T}$ in the Hilbert-space setting (in which $\vec{B}$ is considered as an operator of multiplication). Nevertheless, H of course satisfies (8.17) with $\mathcal{C} = \mathcal{PT}$ provided that the magnetic field is absent.

One of the goals of this section is to determine the class of boundary matrices $A^\pm$ which preserves the $\mathcal{PT}$-symmetry in the sense above. In other words, since we do not like to think of b as a component of a field governed by the additional equations and to mathematically formalize the action of $\mathcal{T}$ on the field (b is rather a fixed parameter in our Hilbert-space setting), we restrict ourselves to rigorously looking for the property

$$[H_0,\mathcal{PT}] = 0\,; \tag{8.18}$$

boundary conditions (8.6) satisfying this relation will be called $\mathcal{PT}$-symmetric. In other words, boundary conditions are $\mathcal{PT}$-symmetric if, and only if, $\mathcal{PT}\Psi$ satisfies the same equations as Ψ in (8.6). Similarly, we shall define $\mathcal{PK}$-symmetric boundary conditions.

In our one-dimensional situation (8.5), the parity $\mathcal{P}$ and the time reversal operator $\mathcal{T}$ act on spinors as follows (*cf* [25, §30] and [25, §60], respectively)

$$(\mathcal{P}\Psi)(x) := \Psi(-x)\,, \qquad (\mathcal{T}\Psi)(x) := i\sigma_2\overline{\Psi(x)} = \begin{pmatrix} \overline{\psi_-(x)} \\ -\overline{\psi_+(x)} \end{pmatrix}. \tag{8.19}$$

It is important to stress that $\mathcal{T}$ differs from the complex conjugation operator

$$(\mathcal{K}\Psi)(x) := \overline{\Psi(x)}\,, \tag{8.20}$$

the latter being the time reversal operator in the scalar case.

It is easily seen that $\mathcal{P}$, $\mathcal{T}$ and $\mathcal{K}$ are norm-preserving, mutually commuting bijections on $\mathcal{H}$. $\mathcal{P}$ is linear, while $\mathcal{T}$ and $\mathcal{K}$ are antilinear (*i.e.* conjugate-linear) operators. $\mathcal{P}$ and $\mathcal{K}$ are involutive (*i.e.* $\mathcal{P}^2 = 1 = \mathcal{K}^2$), while $\mathcal{T}$ satisfies (8.3).

Proposition 8.2. *H_0 is*

- *$\mathcal{PT}$-symmetric if, and only if, $A^- = \mathcal{T}A^+\mathcal{T}$,* i.e.,

$$A^- = \begin{pmatrix} -\overline{a_{22}} & \overline{a_{21}} \\ \overline{a_{12}} & -\overline{a_{11}} \end{pmatrix} \qquad \textit{for} \qquad A^+ = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} ;$$

- *$\mathcal{PK}$-symmetric if, and only if, $A^- = -\mathcal{K}A^+\mathcal{K} \equiv -\overline{A^+}$,* i.e.,

$$A^- = \begin{pmatrix} -\overline{a_{11}} & -\overline{a_{12}} \\ -\overline{a_{21}} & -\overline{a_{22}} \end{pmatrix} \qquad \textit{for} \qquad A^+ = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} .$$

Proof. Since the space $H^2((-a,a);\mathbb{C}^2)$ is left invariant under the actions of $\mathcal{P}$, $\mathcal{T}$ and $\mathcal{K}$, it is enough to impose algebraic conditions on $A^\pm$ so that the symmetry properties are ensured. More specifically, we need to ensure that $\Psi \in \mathsf{D}(H_0)$ implies $\mathcal{PT}\Psi \in \mathsf{D}(H_0)$. Employing the identity

$$\begin{aligned}(\mathcal{PT}\Psi)'(\pm a) + A^\pm(\mathcal{PT}\Psi)(\pm a) &= (-\mathcal{T}\Psi)'(\mp a) + A^\pm(\mathcal{T}\Psi)(\mp a) \\ &= -\mathcal{T}\left[\Psi'(\mp a) + \mathcal{T}A^\pm\mathcal{T}\Psi(\mp a)\right]\end{aligned}$$

and the bijectivity of $\mathcal{T}$, the $\mathcal{PT}$-symmetry condition follows. The $\mathcal{PK}$-symmetry condition can be established in the same manner. □

Another property we would like to examine in this section is related to the notion of *S-self-adjointness*. We say that a densely defined operator H on a Hilbert space is S-self-adjoint if

$$H^* = S^{-1}HS \tag{8.21}$$

for some bounded and boundedly invertible (possibly antilinear) operator S, where H^* denotes the adjoint of H. It clearly generalizes the notion of self-adjointness and pseudo-Hermiticity.

Proposition 8.3. *H_0 is*

- *self-adjoint if, and only if, $(A^\pm)^* = A^\pm$;*
- *$\mathcal{P}$-self-adjoint if, and only if, $A^- = -(A^+)^*$,* i.e.,

$$A^- = \begin{pmatrix} -\overline{a_{11}} & -\overline{a_{21}} \\ -\overline{a_{12}} & -\overline{a_{22}} \end{pmatrix} \qquad \textit{for} \qquad A^+ = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} ;$$

- *$\mathcal{T}$-self-adjoint if, and only if, $(A^\pm)^* = -\mathcal{T}A^\pm\mathcal{T}$,* i.e.,

$$A^\pm = \begin{pmatrix} a^\pm & 0 \\ 0 & a^\pm \end{pmatrix} \qquad \textit{with} \qquad a^\pm \in \mathbb{C} ;$$

- *$\mathcal{K}$-self-adjoint if, and only if, $(A^\pm)^* = \mathcal{K}A^\pm\mathcal{K} \equiv \overline{A^\pm}$;*

Proof. The claims follows by using similar arguments as in the proof of Proposition 8.2. □

The spectral analysis of non-self-adjoint operators is more difficult than in the self-adjoint case, partly because the *residual spectrum* is in general not empty for the former. One of the goals of the present paper is to point out that the existence of this part of spectrum is always ruled out for S-self-adjoint operators with antilinear S.

Proposition 8.4 (General fact)**.** *Let H be a densely defined closed linear operator on a Hilbert space satisfying* (8.21) *with a bounded and boundedly invertible antilinear operator S. Then the residual spectrum of H is empty.*

Proof. Since H is S-self-adjoint, it is easy to see that λ is an eigenvalue of H (with eigenfunction Ψ) if, and only if, $\bar{\lambda}$ is an eigenvalue of H^* (with eigenfunction $S^{-1}\Psi$). It is then clear from the general identity

$$\sigma_{\mathrm{r}}(H) = \left\{\lambda \in \mathbb{C} \mid \bar{\lambda} \in \sigma_{\mathrm{p}}(H^*) \ \& \ \lambda \notin \sigma_{\mathrm{p}}(H)\right\}$$

that the residual spectrum of H must be empty. □

The proposition generalizes the fact pointed out in [7] for S-self-adjoint operators with S being a conjugation operator (*e.g.* $\mathcal{K}$) and applies to our (different) choice of $\mathcal{T}$.

8.6 Spectral analysis

8.6.1 Location of the spectrum and pseudospectrum

As a consequence of Proposition 8.1, we know that the numerical range of H_b is contained in a sector of the complex plane. Since the spectrum is a subset of the closure of the numerical range, it provides a basic information on the location of the spectrum of H_b. However, coming back to the inequality (8.14) on which the proof of Lemma 8.1 is based, we are able to establish a better result in our case.

Proposition 8.5. *The spectrum of H_b is enclosed in a parabola,*

$$\sigma(H_b) \subset \Xi_b := \left\{ z \in \mathbb{C} \;\middle|\; \Re z \geq -\left(|b| + 4\,|A|^2 + \frac{|A|}{2a} \right) =: C\,, \right.$$
$$\left. |\Im z| \leq \sqrt{8}\,|A|\,\sqrt{\Re z + C} + \frac{|A|}{2a} \right\},$$

where $|A| := |A^+| + |A^-|$.

Proof. By [18, Corol. VI.2.3], the numerical range of H_b is a dense subset of the numerical range of its form h_b, the latter being defined as the set of all complex numbers $h_b[\Psi]$ where Ψ changes over all $\Psi \in \mathsf{D}(h_b)$ such that $\|\Psi\| = 1$. Using the first inequality of (8.14), we get

$$\begin{aligned}
\Re h_b[\Psi] &\geq q_1[\Psi] + b\,q_2[\Psi] - |q_3[\Psi]| \\
&\geq \|\Psi'\|^2 - |b|\,\|\Psi\|^2 - 2\,|A|\,\|\Psi'\|\,\|\Psi\| - \frac{|A|}{2a}\,\|\Psi\|^2 \\
&\geq \frac{1}{2}\,\|\Psi'\|^2 - \left(|b| + 4\,|A|^2 + \frac{|A|}{2a} \right) \|\Psi\|^2\,, \\
|\Im h_b[\Psi]| &\leq |q_3[\Psi]| \leq 2\,|A|\,\|\Psi'\|\,\|\Psi\| + \frac{|A|}{2a}\,\|\Psi\|^2\,,
\end{aligned}$$

for every $\Psi \in \mathsf{D}(h_b)$. The claim follows by combining these two estimates. □

Thus the resolvent set of H_b contains the complement of Ξ_b in $\mathbb{C}$. As a further consequence, we can establish an upper bound on the norm of the resolvent:

$$\|(H_b - z)^{-1}\| \leq 1/\mathrm{dist}\,(z, \partial\Xi_b) \qquad \text{for all} \quad z \in \mathbb{C} \setminus \Xi_b.$$

This result can be also interpreted as a location of the *pseudospectrum* of H_b, *cf* [11, Sec. 9.3].

Remark 8.1. Note that the set Ξ_b in Proposition 8.5 is not symmetric with respect to the real axis. On the other hand, if H_b is $\mathcal{C}$-symmetric with antiunitary $\mathcal{C}$ (*e.g.*, if H_b is $\mathcal{PK}$-symmetric), then we *a priori* know that the numerical range must be symmetric with respect to the real axis and an improved version of Proposition 8.5 holds.

8.6.2 The nature of the spectrum

Since the Neumann Laplacian H_0^N has compact resolvent and the relative bound in Lemma 8.1 can be chosen less than 1/2 (in fact, arbitrarily small), it follows from [18, Thm. VI.3.4] that H_b has compact resolvent as well (for any choice of $A^\pm$).

Proposition 8.6. *H_b has a purely discrete spectrum (*i.e. *any point in the spectrum is an isolated eigenvalue of finite algebraic multiplicity).*

Solving the eigenvalue problem $H_b\Psi = \lambda\Psi$ consists in constructing the fundamental system of $-\psi_\pm'' = k_\pm^2\psi_\pm$ (say, in terms of sines and cosines), with $k_\pm := \sqrt{\lambda \mp b}$, and subject it to the boundary conditions (8.6). This leads to the following algebraic equation for the eigenvalues λ:

$$\begin{aligned}
&\left[\det(A^+) + \det(A^-) - a_{11}^+ a_{22}^- - a_{22}^+ a_{11}^-\right] k_- k_+ \cos(ak_-)\cos(ak_+) \\
&+ \left[\det(A^+)\det(A^-) + a_{11}^+ a_{11}^- k_-^2 + a_{22}^+ a_{22}^- k_+^2 + k_-^2 k_+^2\right] \sin(ak_-)\sin(ak_+) \\
&+ \left[-\det(A^+) a_{22}^- + a_{22}^+ \det(A^-) + (-a_{11}^+ + a_{11}^-) k_-^2\right] k_+ \sin(ak_-)\cos(ak_+) \\
&+ \left[-\det(A^+) a_{11}^- + a_{11}^+ \det(A^-) + (-a_{22}^+ + a_{22}^-) k_+^2\right] k_- \cos(ak_-)\sin(ak_+) \\
&+ \left(a_{21}^+ a_{12}^- + a_{12}^+ a_{21}^-\right) k_- k_+ = 0,
\end{aligned} \tag{8.22}$$

where a_{ij}^+ and a_{ij}^- denote the elements of the matrices A^+ and A^-, respectively.

There are only a few choices of $A^\pm$ for which (8.22) admits explicit solutions. In the sequel we consider some particular situations that we analyse with help of numerical solutions.

8.6.3 Examples

A self-adjoint example with avoided crossings. Let us choose

$$A^{\pm} := \begin{pmatrix} 0 & \mathrm{i}\alpha \\ -\mathrm{i}\alpha & 0 \end{pmatrix}, \tag{8.23}$$

where α is a real parameter. It follows from Proposition 8.3 that all the eigenvalues are real since H_b is self-adjoint. The implicit equation for the eigenvalues takes form

$$2\alpha^2 k_+ k_- [1 - \cos(2ak_+)\cos(2ak_-)] = -(k_+^2 k_-^2 + \alpha^4)\sin(2ak_+)\sin(2ak_-).$$

The dependence of eigenvalues on the parameter α can be seen in Figure 8.1.

An interesting phenomenon in this figure is the approaching of a pair of eigenvalues and its subsequent moving back and slowly approaching to constant values. It should be noted that in the point of closest approach the two curves do not intersect. This avoided crossing holds for each pair of the eigenvalues. In this context, let us recall that the existence of gaps between eigenvalues of self-adjoint operators (which is the case of the present example) is important for the usage of quantum adiabatic theorem (see, *e.g.*, [33]).

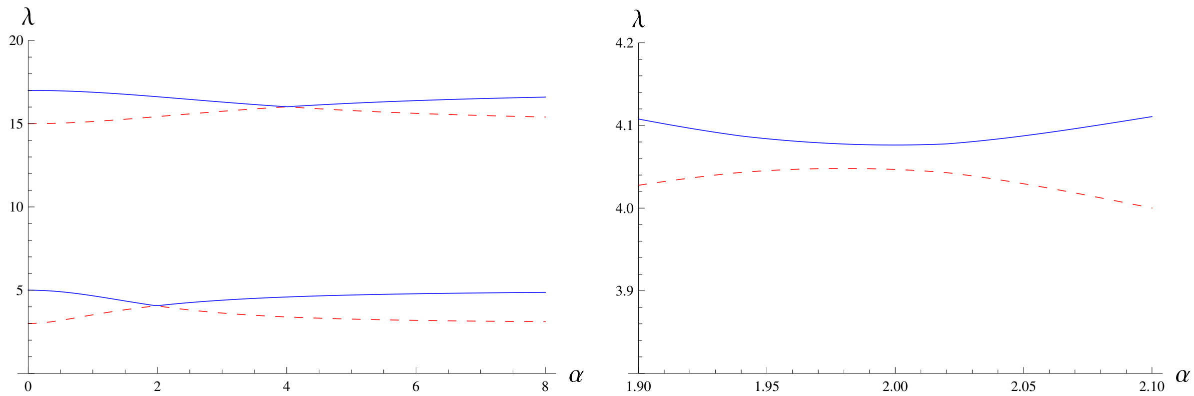

Figure 8.1: α-dependence of eigenvalues for $b = 1$ and $a = \frac{\pi}{4}$ in example (8.23), with a zoom of the avoided crossing of the first pair of eigenvalues on the right.

A $\mathcal{PT}$-symmetric example with real and complex spectra. As an example of non-Hermitian but $\mathcal{PT}$-symmetric boundary conditions, let us consider

$$A^{\pm} = \begin{pmatrix} \mathrm{i}\alpha \pm \beta & 0 \\ 0 & \mathrm{i}\alpha \pm \beta \end{pmatrix}, \tag{8.24}$$

where α and β are real parameters. The feature of this example is that the spinorial components do not mix. The implicit equation for the eigenvalues acquires the form

$$\begin{aligned} &\big(-2\beta k_- \cos(2ak_-) + (k_-^2 - \alpha^2 - \beta^2)\sin(2ak_-)\big) \\ &\qquad \times \big(-2\beta k_+ \cos(2ak_+) + (k_+^2 - \alpha^2 - \beta^2)\sin(2ak_+)\big) = 0. \end{aligned} \tag{8.25}$$

Because of the decoupling, this eigenvalue problem can be analysed by using known results for this type of boundary conditions in the scalar case previously studied in [21] and in more detail in [22]. It turns out that the spectrum significantly depends on the sign of β.

$\underline{\beta = 0}$. It follows from [21] that one pair of eigenvalues depend on the parameter α quadratically and the others are constant, see the left part of Figure 8.2. More specifically, the eigenvalues explicitly read

$$\lambda_{j,\pm} = \begin{cases} \alpha^2 \mp b & \text{if} \quad j = 0\,, \\ \left(\frac{j\pi}{2a}\right)^2 \mp b & \text{if} \quad j \geq 1\,. \end{cases} \tag{8.26}$$

The crossings of full (respectively dashed) lines in the left part of Figure 8.2 correspond to eigenvalues of geometric multiplicity one and algebraic multiplicity two, while the crossings of full lines with dashed lines

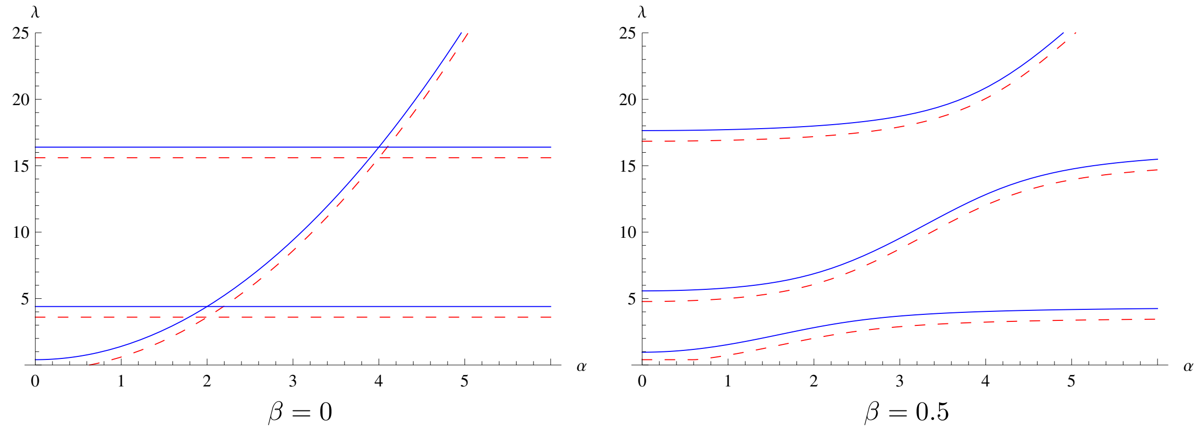

Figure 8.2: α-dependence of eigenvalues for $b = 0.4$ and $a = \frac{\pi}{4}$ in example (8.24).

correspond to eigenvalues of both multiplicities equal to two. The entire spectrum is doubly degenerate for $b = 0$ and there exist eigenvalues of geometric multiplicity two and algebraic multiplicity four.

$\beta > 0$. In this case, the reality of the spectrum was proved in [22]. The right part of Figure 8.2 shows the dependence of the eigenvalues on the parameter α. We again observe pairs of eigenvalues split because of the presence of the magnetic field.

$\beta < 0$. On the other hand, the reality of the spectrum in the case when β is negative is not guaranteed and, indeed, it is easily seen from Figure 8.3 that complex conjugate pairs of eigenvalues do appear when a couple of real eigenvalues collides as enlarging α. The pair of complex eigenvalues becomes real again for larger values of α. It follows from the analysis in [22] that only one pair of complex conjugate eigenvalues occurs simultaneously in the spectrum.

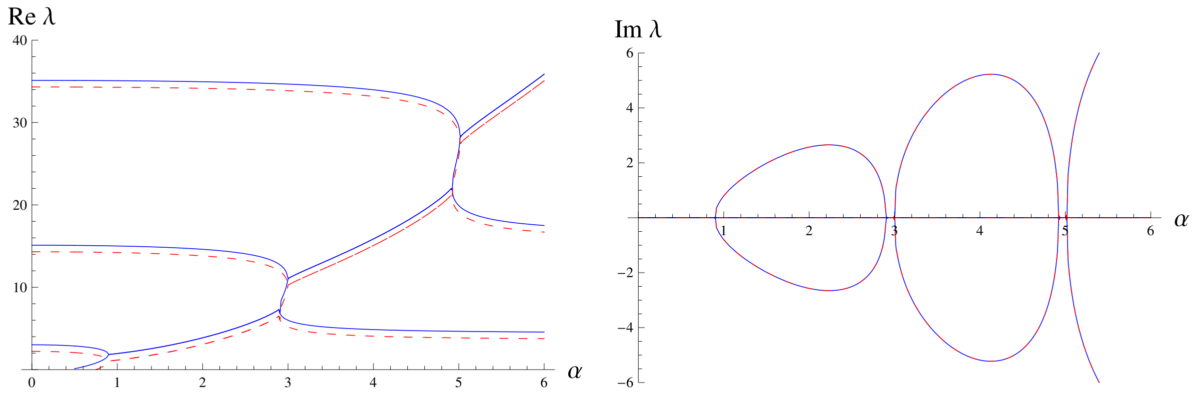

Figure 8.3: α-dependence of the real (left) and imaginary (right) parts of eigenvalues for $b = 0.4$, $a = \frac{\pi}{4}$ and $\beta = -0.5$ in example (8.24).

Note that the choice (8.24) with $\beta = 0$ fits exactly into the scattering setting treated in Section 8.3. An alternative physical interpretation of the model (8.24) can be given in terms of the metric approach discussed in Section 8.7 below.

A $\mathcal{PT}$-symmetric example with coupled spinorial components As another example of non-Hermitian $\mathcal{PT}$-symmetric boundary conditions, let us select

$$A^{\pm} = \begin{pmatrix} 0 & \pm i\alpha \\ \pm i\alpha & 0 \end{pmatrix}, \tag{8.27}$$

where α is a real parameter. The characteristic feature of this model is a non-trivial mixing of spinorial components. The implicit equation for the eigenvalues now takes the form

$$\begin{aligned} 4\alpha^2 k_+ k_- \cos(ak_+)^2 \cos(ak_-)^2 + 4\alpha^2 k_+ k_- \sin(ak_+)^2 \sin(ak_-)^2 \\ = -(k_+ k_- + \alpha^4) \sin(2ak_+) \sin(2ak_-). \end{aligned} \tag{8.28}$$

The dependence of low-lying eigenvalues on the parameter α can be seen in Figure 8.4. Here the lowest pair of real eigenvalues exhibits a crossing. However, the eigenvalues remain real after the crossing point as the parameter α increases. This behaviour is not featured uniquely by the lowest pair of eigenvalues, it also appears for higher-lying eigenvalues in the spectrum (not visible in the figure). On the other hand, as α increases, the other pairs of eigenvalues in the figure complexify after the first collision, then the corresponding eigenvalues propagate as complex conjugate pairs in the complex plane, meet again and become real.

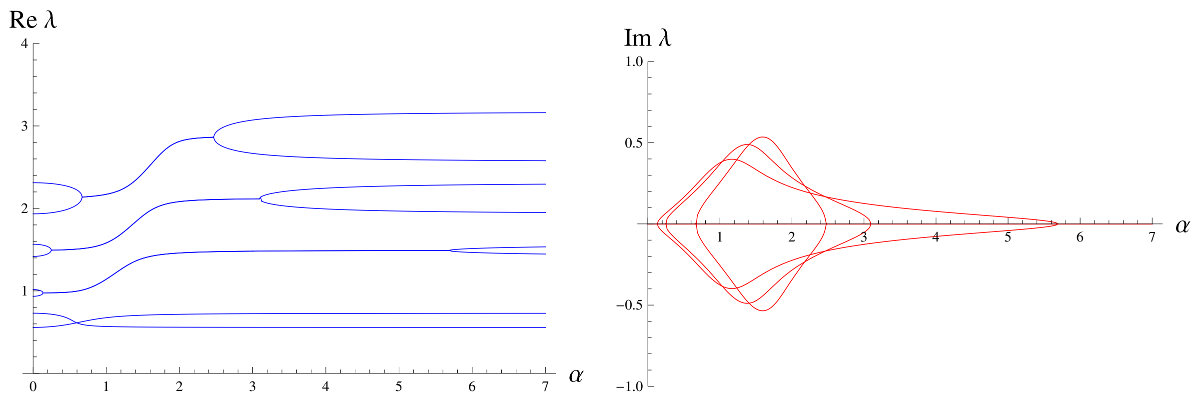

Figure 8.4: α-dependence of eigenvalues for $b = 0.5$, $a = \sqrt{43}$ in example (8.27). An animation can be found on the website [19].

8.7 Conclusions

The goal of this paper was to investigate the role of spin in complex extensions of quantum mechanics on a simple model of Pauli equation with complex Robin-type boundary conditions. A special attention was paid to $\mathcal{PT}$-symmetric situations with a physical choice of the time-reversal operator $\mathcal{T}$.

A simple physical interpretation of our model in terms of scattering was suggested in Section 8.3. It would be desirable to examine this motivation in more details and include "spin-dependent electric potential" (*e.g.* Bychkov-Rashba or Dreselhauss spin-orbit terms typical for semiconductor physics [14]).

Robin boundary conditions represent a class of separated boundary conditions. Our model can be naturally extended to connected boundary conditions, whose spectral analysis represents a direction of potential future research (*cf* [22, 12, 13] in the scalar case).

In this paper we did not discuss the important question of the existence of similarity transformations (or the "metric" in the $\mathcal{PT}$-symmetric context) connecting our non-Hermitian operators with self-adjoint Hamiltonians. The problem generally constitutes a difficult task and very few closed formulae are known (*cf* [20, 3, 2, 23] and references therein). However, we can easily extend the results established in the scalar case without magnetic field [23] to our spinorial example (8.24) and compute the metric in this special case. Let us define

$$\Theta := \begin{pmatrix} I+K & 0 \\ 0 & I+K \end{pmatrix},$$

where I denotes the identity operator on $L^2((-a,a))$ and K is an integral operator with kernel

$$K(x,y) := e^{\mathrm{i}\alpha(x-y)-\beta|x-y|}\left[c + \mathrm{i}\alpha\,\mathrm{sgn}(x-y)\right],$$

with c being any real number. It follows from [23, Sec. 4.5] and the nature of the decoupled boundary conditions (8.24) that Θ represents a one-parametric family of metrics for H_b under the $\mathcal{PT}$-symmetric choice (8.24). More precisely, H_b is Θ^{-1}-self-adjoint (*cf* (8.21)) and Θ is *positive* provided that either: a is small; or β is positive and large; or $|c|$ and $|\alpha|$ are small. To find the self-adjoint counterpart of H_b determined by this similarity transformation constitutes an open problem (in the scalar case [23] there exists results for $\beta = 0$).

Our model was effectively one-dimensional. Higher dimensional generalizations in the spirit of [7, 8, 30] would be especially interesting for variable boundary conditions (*i.e.* non-constant matrix A).

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Chapter 9

Spectral analysis of the diffusion operator with random jumps from the boundary

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Spectral analysis of the diffusion operator with random jumps from the boundary

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Abstract. Using an operator-theoretic framework in a Hilbert-space setting, we perform a detailed spectral analysis of the one-dimensional Laplacian in a bounded interval, subject to specific non-self-adjoint connected boundary conditions modelling a random jump from the boundary to a point inside the interval. In accordance with previous works, we find that all the eigenvalues are real. As the new results, we derive and analyse the adjoint operator, determine the geometric and algebraic multiplicities of the eigenvalues, write down formulae for the eigenfunctions together with the generalised eigenfunctions and study their basis properties. It turns out that the latter heavily depend on whether the distance of the interior point to the centre of the interval divided by the length of the interval is rational or irrational. Finally, we find a closed formula for the metric operator that provides a similarity transform of the problem to a self-adjoint operator.

9.1 Introduction

In this paper we are interested in the non-self-adjoint eigenvalue problem

$$\begin{cases} -\psi'' = \lambda\psi \qquad \text{in} \qquad (-\frac{\pi}{2}, \frac{\pi}{2})\,, \\ \psi(\pm\frac{\pi}{2}) = \psi(\frac{\pi}{2}a)\,, \end{cases} \tag{9.1}$$

with a real parameter $a \in (-1, 1)$. The operator H associated with (9.1) is the generator of the following stochastic process:

1. Start a Brownian motion with quadratic variation equal to 2 in the interval $(-\frac{\pi}{2}, \frac{\pi}{2})$ and wait until it hits one of the boundary points $\pm\frac{\pi}{2}$.
2. At the hitting time of $\pm\frac{\pi}{2}$ the Brownian particle gets restarted in an interior point $\frac{\pi}{2}a$ and repeats the process at the previous step.

This process is sometimes described as the Brownian motion on the figure eight [8]. The existence of such a process is in fact elementary and it can be constructed by piecing together Brownian motions in a rather direct way. The problem (9.1) can be also understood as a spectral problem for a non-self-adjoint graph with regular boundary conditions [9].

There are several obvious generalisations of the stochastic process. Firstly, instead of restarting the process at the fixed point $\frac{\pi}{2}a$, one could restart it according to a given probability distribution μ on $(-\frac{\pi}{2}, \frac{\pi}{2})$. Secondly, one can even take two different probability distributions μ_- and μ_+ on $(-\frac{\pi}{2}, \frac{\pi}{2})$ and restart the process according to $\mu_\pm$ depending on whether the boundary point $\pm\frac{\pi}{2}$ has been hit. This generalised process leads to the following analogue of (9.1):

$$\begin{cases} -\psi'' = \lambda\psi \qquad \text{in} \qquad (-\frac{\pi}{2}, \frac{\pi}{2})\,, \\ \psi(\pm\frac{\pi}{2}) = \displaystyle\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} \psi(x)\,\mu_\pm(dx)\,. \end{cases} \tag{9.2}$$

Despite its apparent simplicity, the process leads to several interesting results. First of all, it has been shown by Leung et al. in [16] that, even in the most general setting described above, the spectrum of the operator H^{μ_-,μ_+} associated with (9.2) is purely real, a property which cannot be typically expected for non-selfadjoint operators. It has also been shown in [16], that the spectral gap of H^{μ_-,μ_+} is always greater than the first Dirichlet eigenvalue of the Laplacian in the interval $(-\frac{\pi}{2}, \frac{\pi}{2})$. Furthermore, it has been shown analytically in [16] and probabilistically in [11] that in the case of $\mu_+ = \mu_-$ the spectral gap of the spectrum of the generator H^{μ_-,μ_+} always coincides with the second Dirichlet eigenvalue of the Laplacian in the interval $(-\frac{\pi}{2}, \frac{\pi}{2})$, independently of the specific choice of $\mu_+ = \mu_-$.

Thus it is fair to say that this family of non-selfadjoint differential operators exhibits rich spectral features. This is our starting point and we aim to further develop some of the spectral-theoretic properties of members of this family of non-self-adjoint differential operators.

In this paper we are concerned with the most simple case (9.1) and investigate the associated operator H from a purely spectral-theoretic perspective and complement existing results which mainly focused on the determination of eigenvalues or even only on the spectral gap. We investigate the spectrum of the operator H and its adjoint H^*, determine algebraic multiplicities of the eigenvalues and analyse the basis properties of the set of eigenfunctions. Due to the non-self-adjointness of the operator, it is not at all clear in which sense the eigenfunctions can be expected to be a basis of the associated Hilbert space. In these respects we further develop certain strands of research first developed in [8], whose authors calculated among other things the spectrum of the above operator in the case $a = 0$; see also [3] and [4], where the authors derive results on the spectrum of the above operator including geometric multiplicities of the eigenvalues.

The organisation of this paper is as follows. In Section 9.2 we properly define H as a closed operator in the Hilbert space $L^2((-\frac{\pi}{2}, \frac{\pi}{2}))$ and state its basic properties. We also provide an *a priori* proof of the reality of the eigenvalues of H, without the need to compute the eigenvalues and eigenfunctions explicitly. The latter is done only in Section 9.3, where we analyse geometric degeneracies of the eigenvalues (Proposition 9.1). In Section 9.4 we find the adjoint operator H^* and compute its spectrum (Proposition 9.2). These results enable us in Section 9.5 to eventually determine algebraic degeneracies of the eigenvalues of H (Proposition 9.4). It turns out that the eigenvalue degeneracies heavily depend on Diophantine properties of the parameter a.

Theorem 9.1. *All the eigenvalues of H are algebraically simple if, and only if, $a \notin \mathbb{Q}$.*

In the second part of the paper, namely in Section 9.7, we study basis properties of H. Using the explicit knowledge of the resolvent kernel of H constructed in Section 9.6, we first show in Section 9.7.1 that the eigenfunctions together with the generalised eigenfunctions form a complete set in $L^2((-\frac{\pi}{2}, \frac{\pi}{2}))$. Then we study the minimal completeness and conditional-basis properties in Sections 9.7.2 and 9.7.3, respectively. These results can be summarised as follows.

Theorem 9.2.

1. *If $a \notin \mathbb{Q}$, then the eigenfunctions of H form a minimal complete set but not a conditional basis in $L^2((-\frac{\pi}{2}, \frac{\pi}{2}))$.*

2. *If $a \in \mathbb{Q}$, then the eigenfunctions of H do not form a minimal complete set in $L^2((-\frac{\pi}{2}, \frac{\pi}{2}))$.*

Finally, in Section 9.7.4, we are interested in the possibility of the quasi-self-adjointness relation

$$H^*\Theta = \Theta H \,, \tag{9.3}$$

where Θ is a positive operator called a *metric*. The concept of quasi-self-adjoint operators goes back to a seminal paper of Dieudonné [6] and has been renewed recently in the context of quantum mechanics with non-self-adjoint operators; we refer to [14] and [13, Chap. 5] for more details and references.

Theorem 9.3. *Let $a \notin \mathbb{Q}$. The operator H satisfies the relation* (9.3) *with the operator Θ explicitly given by* (9.63). *The latter is a positive, bounded and invertible operator (the inverse is unbounded).*

In view of this theorem, the reality of the spectrum of H can be understood as a consequence of a generalised similarity to a self-adjoint operator. We would like to emphasise that we have an explicit and particularly simple formula (9.63) for the metric operator Θ. There are not many non-self-adjoint models in the literature for which the metric operator can be constructed in a closed form, *cf* [15] and references therein.

We conclude the paper by Section 9.8 where we suggest some open problems.

9.2 An operator-theoretic setting and basic properties

We understand (9.1) as a spectral problem for the operator H in $L^2((-\frac{\pi}{2}, \frac{\pi}{2}))$ defined by

$$H\psi := -\psi'' \,, \qquad \psi \in \mathsf{D}(H) := \left\{ \psi \in H^2((-\tfrac{\pi}{2}, \tfrac{\pi}{2})) \;\middle|\; \psi(-\tfrac{\pi}{2}) = \psi(\tfrac{\pi}{2}a) = \psi(\tfrac{\pi}{2}) \right\} . \tag{9.4}$$

Note that the boundary values are well defined due to the embedding $H^2((-\frac{\pi}{2}, \frac{\pi}{2})) \hookrightarrow C^1([-\frac{\pi}{2}, \frac{\pi}{2}])$.

Let us first state some basic properties of H. In the sequel, $\|\cdot\|$ and $(\cdot, \cdot)$ denote respectively the norm and inner product (antilinear in the first argument) of the Hilbert space $L^2((-\frac{\pi}{2}, \frac{\pi}{2}))$.

- H is **densely defined** because $C_0^\infty\big((-\frac{\pi}{2}, \frac{\pi}{2}) \setminus \{\frac{\pi}{2}a\}\big) \subset \mathsf{D}(H)$ and $C_0^\infty\big((-\frac{\pi}{2}, \frac{\pi}{2}) \setminus \{\frac{\pi}{2}a\}\big)$ is dense in $L^2\big((-\frac{\pi}{2}, \frac{\pi}{2}) \setminus \{\frac{\pi}{2}a\}\big) \simeq L^2((-\frac{\pi}{2}, \frac{\pi}{2}))$.

- H is **closed**, which can be directly shown as follows. First of all, let us notice that there exists a positive constant C such that
$$\forall \psi \in \mathsf{D}(H)\,, \qquad \|\psi'\|^2 \leq C\,(\|\psi\|^2 + \|\psi''\|^2)\,. \tag{9.5}$$
Indeed, integrating by parts and using the boundary conditions, we find
$$\begin{aligned}\|\psi'\|^2 &= (\psi, -\psi'') + \bar{\psi}(\tfrac{\pi}{2}a)\left[\psi'(\tfrac{\pi}{2}) - \psi'(-\tfrac{\pi}{2})\right] \\ &= (\psi, -\psi'') + \bar{\psi}(\tfrac{\pi}{2}a)\,(1, \psi'') \\ &\leq \|\psi\|\|\psi''\| + |\psi(\tfrac{\pi}{2}a)|\,\sqrt{\pi}\,\|\psi''\|\,,\end{aligned}$$
where the last line is due to the Schwarz inequality. At the same time, by quantifying the embedding $H^1((-\frac{\pi}{2}, \frac{\pi}{2})) \hookrightarrow C^0([-\frac{\pi}{2}, \frac{\pi}{2}])$, we have
$$|\psi(x)|^2 \leq \frac{1}{\pi}\,\|\psi\|^2 + 2\,\|\psi\|\|\psi'\| \leq \left(\frac{1}{\pi} + \frac{1}{\epsilon}\right)\|\psi\|^2 + \epsilon\,\|\psi'\|^2 \tag{9.6}$$
for every $\psi \in H^1((-\frac{\pi}{2}, \frac{\pi}{2}))$, $x \in [-\frac{\pi}{2}, \frac{\pi}{2}]$ and any $\epsilon > 0$. Putting these two inequalities together, we verify (9.5).
Now, let $\{\psi_n\}_{n=1}^\infty \subset \mathsf{D}(H)$ be such that $\psi_n \to \psi$ and $-\psi_n'' \to \phi$ as $n \to \infty$. Applying (9.5) to ψ_n, we see that $\{\psi_n\}_{n=1}^\infty$ is a bounded sequence in $H^2((-\frac{\pi}{2}, \frac{\pi}{2}))$ and thus weakly converging in this space. Hence, $\psi \in H^2((-\frac{\pi}{2}, \frac{\pi}{2}))$ and $\phi = -\psi''$. Applying (9.5) to $\psi_n - \psi$, we see that $\psi_n \to \psi$ strongly in $H^2((-\frac{\pi}{2}, \frac{\pi}{2}))$ as $n \to \infty$. The preservation of the boundary conditions in the limit is ensured by the embedding inequality (9.6).
- H is **quasi-accretive** (*cf* [10, Sec. V.3.10]). Indeed, for every $\psi \in \mathsf{D}(H)$,
$$\begin{aligned}\Re\,(\psi, H\psi) &= \|\psi'\|^2 - \Re\left[(\bar{\psi}\psi')(\tfrac{\pi}{2}) - (\bar{\psi}\psi')(-\tfrac{\pi}{2})\right] \\ &= \|\psi'\|^2 - \frac{1}{2}\int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} |\psi|^{2\prime}(x)\,dx \\ &\geq \|\psi'\|^2 - \|\psi'\|\|\psi\| \\ &\geq \left(1 - \frac{\epsilon}{4}\right)\|\psi'\|^2 - \frac{1}{4\epsilon}\,\|\psi\|^2\end{aligned}$$
with any $\epsilon > 0$. Choosing $\epsilon = 4$, we see that $H + \frac{1}{16}$ is accretive.
- H has purely **real eigenvalues**. This striking property can be shown *a priori*, without solving the eigenvalue problem explicitly, as follows. Multiplying the first equation in (9.1) by ψ', we arrive at the first integral
$$-\,\psi'^2 - \lambda\psi^2 = \text{const} \qquad \text{in} \qquad (-\tfrac{\pi}{2}, \tfrac{\pi}{2})\,. \tag{9.7}$$
Using the boundary conditions of (9.1), we thus deduce that the derivative of any eigenfunction ψ of H satisfies
$$\psi'(-\tfrac{\pi}{2})^2 = \psi'(\tfrac{\pi}{2}a)^2 = \psi'(\tfrac{\pi}{2})^2\,. \tag{9.8}$$
We divide the analysis into two cases now.
    1. Let $\psi'(\frac{\pi}{2}a) = \psi'(\frac{\pi}{2})$. Then ψ is a solution of the problem $-\psi'' = \lambda\psi$ in $(\frac{\pi}{2}a, \frac{\pi}{2})$, subject to periodic boundary conditions $\psi(\frac{\pi}{2}a) = \psi(\frac{\pi}{2})$ and $\psi'(\frac{\pi}{2}a) = \psi'(\frac{\pi}{2})$. This is a self-adjoint problem and thus $\lambda \in \mathbb{R}$. Actually,
    $$\lambda = \left(\frac{4m}{1-a}\right)^2\,, \qquad m \in \mathbb{N}\,.$$
    The same argument applies to the situation $\psi'(\frac{\pi}{2}a) = \psi'(-\frac{\pi}{2})$, where we find
    $$\lambda = \left(\frac{4m}{1+a}\right)^2\,, \qquad m \in \mathbb{N}\,.$$
    In this paper we use the convention $0 \in \mathbb{N}$ and set $\mathbb{N}^* := \mathbb{N} \setminus \{0\}$.
    2. Let $\psi'(\frac{\pi}{2}a) = -\psi'(\frac{\pi}{2})$. If $\psi'(\frac{\pi}{2}a) = \psi'(-\frac{\pi}{2})$, we are in the previous case for which we already know that the eigenvalues are real. We may thus assume $\psi'(\frac{\pi}{2}a) = -\psi'(-\frac{\pi}{2})$ as well. But then ψ is a solution of the problem $-\psi'' = \lambda\psi$ in the whole interval $(-\frac{\pi}{2}, \frac{\pi}{2})$, subject to periodic boundary conditions $\psi(-\frac{\pi}{2}) = \psi(\frac{\pi}{2})$ and $\psi'(-\frac{\pi}{2}) = \psi'(\frac{\pi}{2})$. This is again a self-adjoint problem and thus $\lambda \in \mathbb{R}$. Actually,
    $$\lambda = (2m)^2\,, \qquad m \in \mathbb{N}\,.$$

The above analysis implies:

$$\sigma_{\mathrm{p}}(H) \subset \left\{ \left(\frac{4m}{1-a}\right)^2, \left(\frac{4m}{1+a}\right)^2, (2m)^2 \right\}_{m\in\mathbb{N}} .$$

The opposite inclusion $\supset$ will follow from an explicit solution of the spectral problem (9.1) (alternatively, we could construct admissible eigenfunctions for (9.1) from the periodic solutions discussed above, but this would be almost like solving (9.1) explicitly).

The fact that the total spectrum of H is real will follow from the reality of the eigenvalues established here, but only after we show that H has a *purely discrete spectrum.* To see the latter, we remark that $\mathsf{D}(H)$ is a subset of $H^2((-\frac{\pi}{2}, \frac{\pi}{2}))$, which is compactly embedded in $L^2((-\frac{\pi}{2}, \frac{\pi}{2}))$. But we still need to show that the resolvent set of H is not empty, in order to show that H is an operator with compact resolvent. To this aim, we shall determine the adjoint of H. First, however, let us study the point spectrum of H in detail.

9.3 The point spectrum

In this section we compute the point spectrum of H by solving the eigenvalue problem (9.1) explicitly. Set $\lambda =: k^2$. The general solution of the differential equation in (9.1) reads (including $\lambda = 0$)

$$\psi(x) = A\sin(kx) + B\cos(kx) , \qquad A, B \in \mathbb{C} .$$

Subjecting this solution to the boundary conditions of (9.1), we arrive at the homogeneous system

$$\begin{pmatrix} \sin(k\frac{\pi}{2}) + \sin(k\frac{\pi}{2}a) & -\cos(k\frac{\pi}{2}) + \cos(k\frac{\pi}{2}a) \\ \sin(k\frac{\pi}{2}) - \sin(k\frac{\pi}{2}a) & \cos(k\frac{\pi}{2}) - \cos(k\frac{\pi}{2}a) \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} . \tag{9.9}$$

Eigenfunctions of (9.1) correspond to non-trivial solutions of this system, which in turn are determined by the singularity condition

$$\begin{vmatrix} \sin(k\frac{\pi}{2}) + \sin(k\frac{\pi}{2}a) & -\cos(k\frac{\pi}{2}) + \cos(k\frac{\pi}{2}a) \\ \sin(k\frac{\pi}{2}) - \sin(k\frac{\pi}{2}a) & \cos(k\frac{\pi}{2}) - \cos(k\frac{\pi}{2}a) \end{vmatrix} = -4\sin\left(k\tfrac{\pi}{4}(1+a)\right)\sin\left(k\tfrac{\pi}{4}(1-a)\right)\sin\left(k\tfrac{\pi}{2}\right) = 0 .$$

Consequently,

$$\sigma_{\mathrm{p}}(H) = \left\{ \left(\frac{4m}{1-a}\right)^2, \left(\frac{4m}{1+a}\right)^2, (2m)^2 \right\}_{m\in\mathbb{N}} . \tag{9.10}$$

It will be convenient to introduce the notation

$$\sigma_{\pm 1} := \left\{ \left(\frac{4m}{1\pm a}\right)^2 \right\}_{m\in\mathbb{N}^*} , \qquad \sigma_0 := \left\{ (2m)^2 \right\}_{m\in\mathbb{N}} , \tag{9.11}$$

and refer to eigenvalues from σ_{+1}, σ_{-1} and σ_0 as eigenvalues from the "+1 class", "−1 class" and "0 class", respectively. Note that zero is excluded from $\sigma_{\pm 1}$ and that the sets σ_{+1}, σ_{-1} and σ_0 are not disjoint in general. Dependence of the eigenvalues on the parameter a is depicted in Figure 9.1.

Now we specify the eigenfunctions associated with the individual classes. To study the eigenfunctions corresponding to the classes ± 1, it is useful to rewrite (9.9) into the form

$$\begin{pmatrix} \sin(k\frac{\pi}{4}(1+a))\cos(k\frac{\pi}{4}(1-a)) & \sin(k\frac{\pi}{4}(1+a))\sin(k\frac{\pi}{4}(1-a)) \\ \sin(k\frac{\pi}{4}(1-a))\cos(k\frac{\pi}{4}(1+a)) & -\sin(k\frac{\pi}{4}(1+a))\sin(k\frac{\pi}{4}(1-a)) \end{pmatrix} \begin{pmatrix} A \\ B \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix} . \tag{9.12}$$

- $\boxed{-1 \text{ class eigenvalues}}$ That is, $k = \frac{4m}{1-a}$ with $m \in \mathbb{N}^*$. In this case, the second equation of (9.12) is automatically satisfied, while the first yields the condition

$$A \sin\left(m\pi\tfrac{1+a}{1-a}\right) = 0 .$$

There are two possibilities:

1. If $m\frac{1+a}{1-a} \notin \mathbb{N}$ (generic situation), then $A = 0$ and the eigenfunction associated with k^2 reads

$$\psi(x) = B\cos\left(\frac{4m}{1-a}x\right) , \tag{9.13}$$

with a normalisation constant $B \in \mathbb{C} \setminus \{0\}$.

2. If $m\frac{1+a}{1-a} \in \mathbb{N}$ (exceptional situation), then there are two (independent) eigenfunctions

$$\psi_1(x) = A \sin\left(\frac{4m}{1-a}x\right), \qquad \psi_2(x) = B \cos\left(\frac{4m}{1-a}x\right), \tag{9.14}$$

with normalisation constants $A, B \in \mathbb{C} \setminus \{0\}$.

- $\boxed{\text{+1 class eigenvalues}}$ That is, $k = \frac{4m}{1+a}$ with $m \in \mathbb{N}^*$. Here the situation is reversed with respect to the previous one. Now the first equation of (9.12) is automatically satisfied, while the second yields the condition

$$A \sin\left(m\pi\frac{1-a}{1+a}\right) = 0 .$$

There are again two possibilities:

1. If $m\frac{1-a}{1+a} \notin \mathbb{N}$ (generic situation), then $A = 0$ and the eigenfunction associated with k^2 reads

$$\psi(x) = B \cos\left(\frac{4m}{1+a}x\right), \tag{9.15}$$

with a normalisation factor $B \in \mathbb{C} \setminus \{0\}$.

2. If $m\frac{1-a}{1+a} \in \mathbb{N}$ (exceptional situation), then there are two (independent) eigenfunctions

$$\psi_1(x) = A \sin\left(\frac{4m}{1+a}x\right), \qquad \psi_2(x) = B \cos\left(\frac{4m}{1+a}x\right), \tag{9.16}$$

with normalisation constants $A, B \in \mathbb{C} \setminus \{0\}$.

- $\boxed{\text{0 class eigenvalues}}$ That is, $k = 2m$ with $m \in \mathbb{N}$. In this case, the two equations of (9.9) reduce to one

$$A \sin(m\pi a) = B\left[\cos(m\pi) - \cos(m\pi a)\right] . \tag{9.17}$$

There are several possibilities:

1. If $m = 0$ (zero eigenvalue), there is just one (constant) eigenfunction

$$\psi(x) = B \in \mathbb{C} \setminus \{0\} . \tag{9.18}$$

2. If and $m \neq 0$ and $ma \notin \mathbb{N}$ (generic situation), then we express A as a function of B and the eigenfunction associated with k^2 reads

$$\psi(x) = B\left[\cos(2mx) + \frac{\cos(m\pi) - \cos(m\pi a)}{\sin(m\pi a)} \sin(2mx)\right], \tag{9.19}$$

with a normalisation constant $B \in \mathbb{C} \setminus \{0\}$.

3. If and $m \neq 0$ and $ma \in \mathbb{N}$ (exceptional situation), then (9.17) reads

$$0 = B\left[\cos(m\pi) - \cos(m\pi a)\right] = -2\,B \sin\left(\frac{m\pi(1+a)}{2}\right) \sin\left(\frac{m\pi(1-a)}{2}\right)$$

and we still distinguish two cases:

(a) If $m(1+a)$ is odd (which necessarily implies that $m(1-a)$ is odd as well), then $B = 0$ and there is just one eigenfunction

$$\psi(x) = A \sin(2mx) , \tag{9.20}$$

with a normalisation constant $A \in \mathbb{C} \setminus \{0\}$.

(b) If $m(1+a)$ is even (which necessarily implies that $m(1-a)$ is even as well), there are two (independent) eigenfunctions

$$\psi_1(x) = A \sin(2mx) , \qquad \psi_2(x) = B \cos(2mx) , \tag{9.21}$$

with normalisation constants $A, B \in \mathbb{C} \setminus \{0\}$.

The exceptional situations in the classes -1, $+1$ and 0 are related. First of all, note that $m\frac{1+a}{1-a} \in \mathbb{N}$, $m\frac{1-a}{1+a} \in \mathbb{N}$ or $ma \in \mathbb{N}$ with some $m \in \mathbb{N}^*$ imply that a is rational. Conversely, let a be rational. Then the sets σ_{-1}, σ_{+1} and σ_0 are not disjoint. Clearly, $\lambda = (\frac{4m_{-1}}{1-a})^2 \in \sigma_{-1}$ with some $m_{-1} \in \mathbb{N}^*$ such that $m_{-1}\frac{1+a}{1-a} \in \mathbb{N}$ if, and only if, $\lambda = (\frac{4m_{+1}}{1+a})^2 \in \sigma_{+1}$ with some $m_{+1} \in \mathbb{N}^*$ such that $m_{+1}\frac{1-a}{1+a} \in \mathbb{N}$. At the same time, if $\lambda = (\frac{4m_{\pm1}}{1\pm a})^2 \in \sigma_{\pm1}$ with some $m_{\pm1} \in \mathbb{N}^*$ such that $m_{\pm1}\frac{1\mp a}{1\pm a} \in \mathbb{N}$, then there exists $m_0 \in \mathbb{N}^*$ such that $\lambda = (2m_0)^2 \in \sigma_0$. On the other hand, if $\lambda = (2m_0)^2 \in \sigma_0$ with some $m_0 \in \mathbb{N}^*$ such that $m_0 a \in \mathbb{N}$ and $m_0(1+a)$ is even (which necessarily implies that $m_0(1-a)$ is even as well), then there exist $m_{\pm1} \in \mathbb{N}^*$ such that $m_{\pm1}\frac{1\mp a}{1\pm a} \in \mathbb{N}$ and $\lambda = (\frac{4m_{\pm1}}{1\pm a})^2 \in \sigma_{\pm1}$. Hence, all the exceptional situations with two independent eigenfunctions coincide with the intersection $\sigma_{-1} \cap \sigma_{+1} = \sigma_{-1} \cap \sigma_{+1} \cap \sigma_0$, which is infinite, and the elements of the intersection correspond to eigenvalues of geometric multiplicity two. However, $\sigma_{-1} \cap \sigma_{+1} \neq \sigma_0$; in fact, $\sigma_0 \setminus (\sigma_{-1} \cup \sigma_{+1})$ also contains an infinite number of elements, which correspond to geometrically simple eigenvalues.

On the other hand, if a is irrational, then the sets σ_{-1} σ_{+1} and σ_0 are mutually disjoint and each point in the spectrum is an eigenvalue of geometric multiplicity one.

Let us summarise the spectral properties into the following proposition.

Proposition 9.1. $\sigma_{\mathrm{p}}(H) = \sigma_{-1} \cup \sigma_{+1} \cup \sigma_0$, *where the sets* σ_{-1}, σ_{+1} *and* σ_0 *are introduced in* (9.11).

1. *If* $a \notin \mathbb{Q}$, *then the sets* σ_{-1} σ_{+1} *and* σ_0 *are mutually disjoint and each point of the point spectrum corresponds to an eigenvalue of* H *of geometric multiplicity one, with the associated eigenfunction* (9.13), (9.15), (9.19) *or* (9.18).

2. *If* $a \in \mathbb{Q}$, *then* $\sigma_{-1} \cap \sigma_{+1} = \sigma_{-1} \cap \sigma_{+1} \cap \sigma_0 \neq \varnothing$. *Each point of* $\sigma_{-1} \cap \sigma_{+1}$ *corresponds to an eigenvalue of* H *of geometric multiplicity two, with the associated eigenfunctions* (9.14) *and* (9.16). *Each point of* $\sigma_{\mathrm{p}}(H) \setminus (\sigma_{-1} \cap \sigma_{+1})$ *corresponds to an eigenvalue of geometric multiplicity one, with the associated eigenfunction* (9.13), (9.15), (9.19), (9.20) *or* (9.21) *or* (9.18) *(zero eigenvalue, associated with the constant function* (9.18), *is always geometrically simple).*

It is expected that the geometrically doubly degenerate eigenvalues in $\sigma_{-1} \cap \sigma_{+1} \cap \sigma_0$ will have algebraic multiplicity three. Indeed, fix $a \in \mathbb{Q}$ and consider a point $\lambda \in \sigma_{-1} \cap \sigma_{+1} \cap \sigma_0$. That is, there exists $l, m, n \in \mathbb{N}$ such that

$$\lambda = \left(\frac{4l}{1-a}\right)^2 = \left(\frac{4m}{1+a}\right)^2 = (2n)^2 .$$

Introducing a small perturbation $a \mapsto a + \varepsilon$, the eigenvalue λ splits into three *distinct* eigenvalues of geometric multiplicity one,

$$\lambda_{-1}(\varepsilon) := \left(\frac{4l}{1-a-\varepsilon}\right)^2 \in \sigma_{-1}\,, \qquad \lambda_{+1}(\varepsilon) := \left(\frac{4m}{1+a+\varepsilon}\right)^2 \in \sigma_{+1}\,, \qquad \lambda_0(\varepsilon) := (2n)^2 \in \sigma_0\,,$$

corresponding to mutually linearly independent eigenfunctions.

To discuss the algebraic degeneracies, we first need to determine the adjoint of H.

9.4 The adjoint operator

Obviously, H is a closed extension of the symmetric operator

$$\begin{aligned} (\dot{H}\psi)(x) &:= -\psi''(x)\,, \qquad x \in (-\tfrac{\pi}{2}, \tfrac{\pi}{2}a) \cup (\tfrac{\pi}{2}a, \tfrac{\pi}{2})\,, \\ \psi \in \mathsf{D}(\dot{H}) &:= H_0^2\big((-\tfrac{\pi}{2}, \tfrac{\pi}{2}a)\big) \oplus H_0^2\big((\tfrac{\pi}{2}a, \tfrac{\pi}{2})\big)\,. \end{aligned}$$

That is, $\dot{H} \subset H$. The adjoint $\dot{H}^*$ of $\dot{H}$ is well known:

$$\begin{aligned} (\dot{H}^*\psi)(x) &= -\psi''(x)\,, \qquad x \in (-\tfrac{\pi}{2}, \tfrac{\pi}{2}a) \cup (\tfrac{\pi}{2}a, \tfrac{\pi}{2})\,, \\ \psi \in \mathsf{D}(\dot{H}^*) &= H^2\big((-\tfrac{\pi}{2}, \tfrac{\pi}{2}a)\big) \oplus H^2\big((\tfrac{\pi}{2}a, \tfrac{\pi}{2})\big)\,. \end{aligned}$$

Since $\dot{H} \subset H \subset \dot{H}^*$, we also have

$$\dot{H} \subset H^* \subset \dot{H}^*\,. \tag{9.22}$$

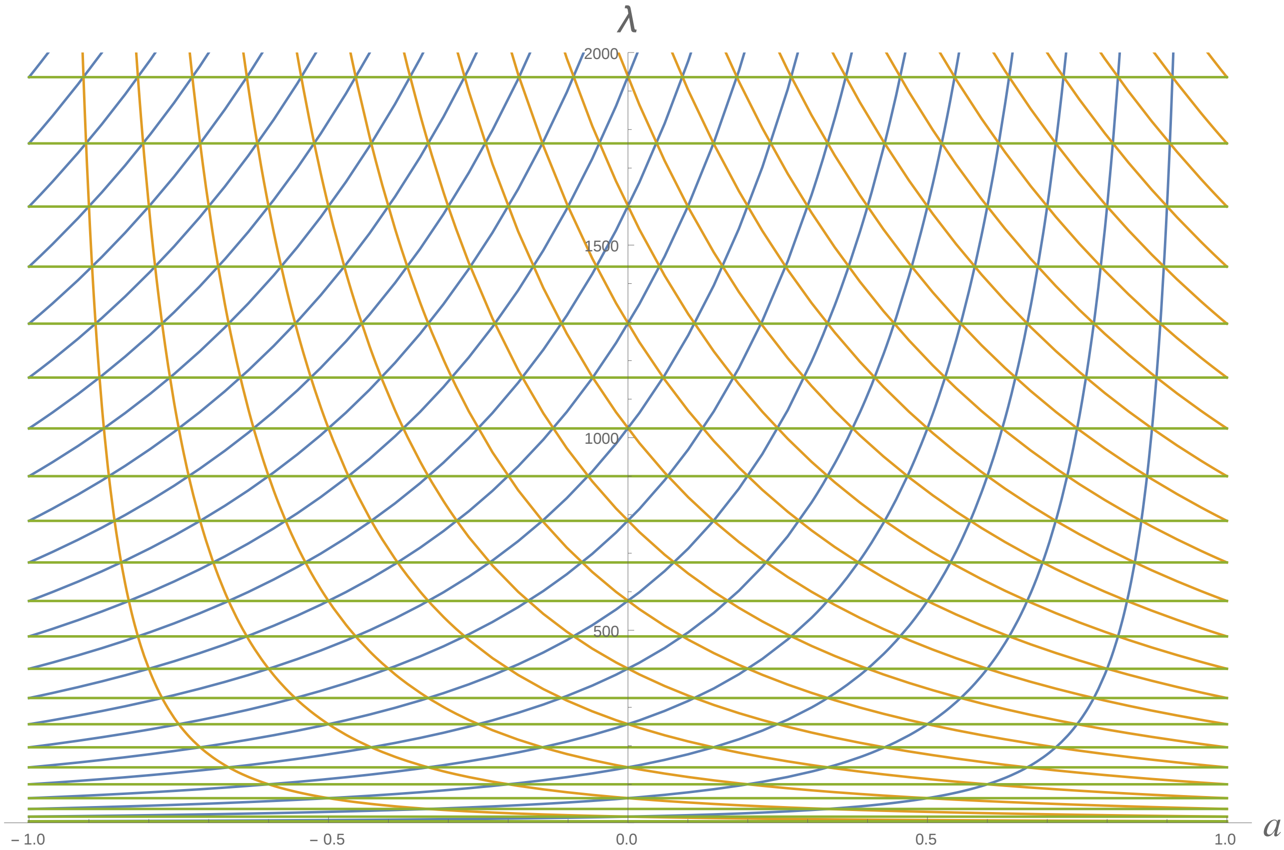

Figure 9.1: Dependence of eigenvalues of H on a. The blue, yellow and green curves correspond to -1, $+1$ and 0 class eigenvalues, respectively, *cf* (9.11). The multiplicities are clearly visible.

It follows that $\mathsf{D}(H^*) \subset H^2\big((-\frac{\pi}{2}, \frac{\pi}{2}a)\big) \oplus H^2\big((\frac{\pi}{2}a, \frac{\pi}{2})\big)$ and that H^* acts as $\dot{H}^*$. Hence, we may integrate by parts to get the identity

$$\begin{aligned}(\phi, H\psi) = (H^*\phi, \psi) &+ \psi(\tfrac{\pi}{2}a)\left[\bar{\phi}'(\tfrac{\pi}{2}a-) - \bar{\phi}'(\tfrac{\pi}{2}a+) + \bar{\phi}'(\tfrac{\pi}{2}) - \bar{\phi}'(-\tfrac{\pi}{2})\right] \\ &+ \psi'(\tfrac{\pi}{2}a)\left[\bar{\phi}(\tfrac{\pi}{2}a+) - \bar{\phi}(\tfrac{\pi}{2}a-)\right] \\ &+ \psi'(-\tfrac{\pi}{2})\bar{\phi}(-\tfrac{\pi}{2}) - \psi'(\tfrac{\pi}{2})\bar{\phi}(\tfrac{\pi}{2})\end{aligned}$$

for every $\psi \in \mathsf{D}(H)$ and $\phi \in \mathsf{D}(\dot{H}^*) \supset \mathsf{D}(H^*)$. Using the arbitrariness of ψ, we thus get

$$(H^*\psi)(x) = -\psi''(x)\,, \qquad x \in (-\tfrac{\pi}{2}, \tfrac{\pi}{2}a) \cup (\tfrac{\pi}{2}a, \tfrac{\pi}{2})\,,$$

$$\psi \in \mathsf{D}(H^*) = \left\{ \psi \in H^2\big((-\tfrac{\pi}{2}, \tfrac{\pi}{2}a)\big) \oplus H^2\big((\tfrac{\pi}{2}a, \tfrac{\pi}{2})\big) \;\middle|\; \begin{array}{c} \phi(-\frac{\pi}{2}) = \phi(\frac{\pi}{2}) = 0 \\ \phi(\frac{\pi}{2}a-) = \phi(\frac{\pi}{2}a+) \\ \phi'(\frac{\pi}{2}) - \phi'(-\frac{\pi}{2}) = \phi'(\frac{\pi}{2}a+) - \phi'(\frac{\pi}{2}a-) \end{array} \right\}.$$

Notice that $\mathsf{D}(H^*) \supset H_0^1((-\frac{\pi}{2}, \frac{\pi}{2}))$.

The point spectrum of H^* can be found by writing down the general solutions of $-\phi'' = k^2\phi$ in $(-\frac{\pi}{2}, \frac{\pi}{2}a)$ and $(\frac{\pi}{2}a, \frac{\pi}{2})$ and subjecting them to the boundary conditions of $\mathsf{D}(H^*)$. Since the procedure is similar to our analysis for H, we just present the results. We find that the eigenvalues of H and H^* coincide, *i.e.*,

$$\sigma_{\mathrm{p}}(H^*) = \sigma_{\mathrm{p}}(H)\,. \tag{9.23}$$

We again use the decomposition $\sigma_{\mathrm{p}}(H^*) = \sigma_{-1} \cup \sigma_{+1} \cup \sigma_0$ and specify the eigenfunctions associated with the individual classes.

- $\boxed{-1 \text{ class eigenvalues}}$ That is, $k = \frac{4m}{1-a}$ with $m \in \mathbb{N}^*$.

  1. If $m\frac{1+a}{1-a} \notin \mathbb{N}$ (generic situation), then the eigenfunction associated with k^2 reads

$$\phi(x) = \begin{pmatrix} 0 \\ A_+ \sin\left(\frac{4m}{1-a}(x - \frac{\pi}{2})\right) \end{pmatrix} \tag{9.24}$$

with a normalisation constant $A_+ \in \mathbb{C}\setminus\{0\}$. Here and in the sequel, for any $\phi = \phi_- \oplus \phi_+ \in L^2((-\frac{\pi}{2}, \frac{\pi}{2}a)) \oplus L^2((\frac{\pi}{2}a, \frac{\pi}{2}))$, we write $\phi = \begin{pmatrix}\phi_- \\ \phi_+\end{pmatrix}$.

2. If $m\frac{1+a}{1-a} \in \mathbb{N}$ (exceptional situation), then there are two (independent) eigenfunctions

$$\phi_1(x) = \begin{pmatrix} 0 \\ A_+ \sin\left(\frac{4m}{1-a}(x-\frac{\pi}{2})\right)\end{pmatrix}, \qquad \phi_2(x) = \begin{pmatrix} A_- \sin\left(\frac{4m}{1-a}(x+\frac{\pi}{2})\right) \\ 0\end{pmatrix}, \tag{9.25}$$

with normalisation constants $A_\pm \in \mathbb{C}\setminus\{0\}$.

- $\boxed{+1 \text{ class eigenvalues}}$ That is, $k = \frac{4m}{1+a}$ with $m \in \mathbb{N}^*$.

1. If $m\frac{1-a}{1+a} \notin \mathbb{N}$ (generic situation), then the eigenfunction associated with k^2 reads

$$\phi(x) = \begin{pmatrix} A_- \sin\left(\frac{4m}{1+a}(x+\frac{\pi}{2})\right) \\ 0\end{pmatrix}, \tag{9.26}$$

with a normalisation constant $A_- \in \mathbb{C}\setminus\{0\}$.

2. If $m\frac{1-a}{1+a} \in \mathbb{N}$ (exceptional situation), then there are two (independent) eigenfunctions

$$\phi_1(x) = \begin{pmatrix} 0 \\ A_+ \sin\left(\frac{4m}{1+a}(x-\frac{\pi}{2})\right)\end{pmatrix}, \qquad \phi_2(x) = \begin{pmatrix} A_- \sin\left(\frac{4m}{1+a}(x+\frac{\pi}{2})\right) \\ 0\end{pmatrix}, \tag{9.27}$$

with normalisation constants $A_\pm \in \mathbb{C}\setminus\{0\}$.

- $\boxed{0 \text{ class eigenvalues}}$ That is, $k = 2m$ with $m \in \mathbb{N}$.

1. If $m = 0$ (zero eigenvalue), there is just one eigenfunction

$$\phi(x) = \begin{pmatrix} C\,(a-1)(x+\frac{\pi}{2}) \\ C\,(a+1)(x-\frac{\pi}{2})\end{pmatrix}, \tag{9.28}$$

with a normalisation constant $C \in \mathbb{C}\setminus\{0\}$.

2. If $m \neq 0$ and $ma \notin \mathbb{N}$ (generic situation), the eigenfunction associated with k^2 reads

$$\phi(x) = \begin{pmatrix} C \sin\left(2m(x+\frac{\pi}{2})\right) \\ C \sin\left(2m(x-\frac{\pi}{2})\right)\end{pmatrix}, \tag{9.29}$$

with a normalisation constant $C \in \mathbb{C}\setminus\{0\}$.

3. If $m \neq 0$ and $ma \in \mathbb{N}$ (exceptional situation), we still distinguish two cases:
   (a) If $m(1+a)$ is odd (which necessarily implies that $m(1-a)$ is odd as well), there is just one eigenfunction, which coincides with (9.29).
   (b) If $m(1+a)$ is even (which necessarily implies that $m(1-a)$ is even as well), there are two (independent) eigenfunctions

$$\phi_1(x) = \begin{pmatrix} 0 \\ A_+ \sin\left(2m(x-\frac{\pi}{2})\right)\end{pmatrix}, \qquad \phi_2(x) = \begin{pmatrix} A_- \sin\left(2m(x+\frac{\pi}{2})\right) \\ 0\end{pmatrix}, \tag{9.30}$$

with normalisation constants $A_\pm \in \mathbb{C}\setminus\{0\}$.

Let us summarise the spectral analysis of H^* into the following proposition.

Proposition 9.2. *$\sigma_{\mathrm{p}}(H^*) = \sigma_{-1} \cup \sigma_{+1} \cup \sigma_0$, where the sets σ_{-1}, σ_{+1} and σ_0 are introduced in* (9.11).

1. *If $a \notin \mathbb{Q}$, then the sets σ_{-1}, σ_{+1} and σ_0 are mutually disjoint and each point of the point spectrum corresponds to an eigenvalue of H^* of geometric multiplicity one, with the associated eigenfunction* (9.24), (9.26), (9.29) *or* (9.28).

2. *If $a \in \mathbb{Q}$, then $\sigma_{-1} \cap \sigma_{+1} = \sigma_{-1} \cap \sigma_{+1} \cap \sigma_0 \neq \varnothing$. Each point of $\sigma_{-1} \cap \sigma_{+1}$ corresponds to an eigenvalue of H^* of geometric multiplicity two, with the associated eigenfunctions* (9.25) *and* (9.27). *Each point of $\sigma_{\mathrm{p}}(H^*) \setminus (\sigma_{-1} \cap \sigma_{+1})$ corresponds to an eigenvalue of geometric multiplicity one, with the associated eigenfunction* (9.24), (9.26), (9.29), (9.30) *or* (9.28) *(zero eigenvalue, associated with the function* (9.28), *is always geometrically simple).*

As the last result of this section, we show that H is an operator with compact resolvent.

Proposition 9.3. *H is a quasi-m-accretive operator with compact resolvent.*

Proof. In Section 9.2, we already showed that $H + \frac{1}{16}$ is accretive. Consequently,

$$\|\psi\|\|(H-z)\psi\| \geq \Re\big(\psi, (H-z)\psi\big) \geq \left(-\Re z - \frac{1}{16}\right)\|\psi\|^2 \tag{9.31}$$

for every $\psi \in \mathsf{D}(H)$ and all $z \in \mathbb{C}$. If $\Re z < -\frac{1}{16}$, this estimate implies that $H - z$ has a bounded inverse with bound not exceeding $1/|\Re z + \frac{1}{16}|$. Hence the range $\mathsf{R}(H-z)$ is closed for all $z \in \Delta := \{z \in \mathbb{C} \mid \Re z < -\frac{1}{16}\}$, so each $z \in \Delta$ does not belong to the continuous nor the point spectrum of H. Using the general characterisation of the residual spectrum (see, *e.g.*, [13, Prop. 5.2.2])

$$\sigma_{\mathrm{r}}(H) = \big\{\lambda \in \mathbb{C} \mid \lambda \notin \sigma_{\mathrm{p}}(H) \;\&\; \overline{\lambda} \in \sigma_{\mathrm{p}}(H^*)\big\}$$

and (9.23), we conclude that $z \in \Delta$ is not in the residual spectrum either. Summing up, no point $z \in \Delta$ belongs to the spectrum of H, so the resolvent exists at every $z \in \Delta$. This together with (9.31) implies that $H + \frac{1}{16}$ is m-accretive. Since $H^2((-\frac{\pi}{2}, \frac{\pi}{2})) \supset \mathsf{D}(H)$ is compactly embedded in $L^2((-\frac{\pi}{2}, \frac{\pi}{2}))$ and the resolvent of H exists at a point (in fact, at every point $z \in \Delta$), we deduce that H is an operator with compact resolvent. □

As a consequence of Proposition 9.3, the spectrum of H (as well as H^*) is purely discrete, in particular, it is exhausted by the eigenvalues (9.10). Summing up,

$$\sigma(H) = \sigma_{-1} \cup \sigma_{+1} \cup \sigma_0 = \sigma(H^*)\,.$$

9.5 Algebraic multiplicities

It is a general fact that $(\phi, \psi) = 0$ is a necessary condition for the existence of a generalised (root) vector for an eigenvalue λ of an operator H, where ψ is a corresponding eigenfunction and ϕ is an eigenfunction of H^* corresponding to $\bar{\lambda}$. The study of algebraic multiplicities of eigenvalues of our operator H is thus reduced to a computation of elementary trigonometric integrals.

- $\boxed{-1 \text{ class eigenvalues}}$ Let $\lambda = \left(\frac{4m}{1-a}\right)^2$ with $m \in \mathbb{N}^*$.
  1. If $m\frac{1+a}{1-a} \notin \mathbb{N}$ (generic situation), we already know that the eigenvalue λ is geometrically simple. The functions ψ and ϕ are given by (9.13) and (9.24), respectively. Since

     $$(\phi, \psi) = -\bar{A}_+ B\,\frac{\pi}{4}\,(1-a)\,\sin\left(m\pi\,\frac{1+a}{1-a}\right)\cos(m\pi) \neq 0\,, \tag{9.32}$$

     the eigenvalue λ is algebraically simple too.
  2. If $m\frac{1+a}{1-a} \in \mathbb{N}$ (exceptional situation), we already know that the eigenvalue λ has geometric multiplicity two. The two eigenfunctions ψ_1, ψ_2 of H and the two eigenfunctions ϕ_1, ϕ_2 of H^* are given by (9.14) and (9.25), respectively. Since

     $$\begin{aligned}(\phi_1, \psi_1) &= \bar{A}_+ A\,\frac{\pi}{4}\,(1-a)\,\cos\left(m\pi\,\frac{1+a}{1-a}\right)\cos(m\pi) \neq 0\,,\\ (\phi_2, \psi_1) &= \bar{A}_- A\,\frac{\pi}{4}\,(1+a)\,\cos\left(m\pi\,\frac{1+a}{1-a}\right)\cos(m\pi) \neq 0\,,\\ (\phi_1, \psi_2) &= 0 = (\phi_2, \psi_2)\,,\end{aligned} \tag{9.33}$$

     there might be a generalised eigenvector ξ of H associated with ψ_2. In fact, the linearly independent solution of $(H - \lambda)\xi = \psi_2$ reads

     $$\xi(x) := -B\,\frac{1-a}{64m^2}\left[(1-a)\,\cos\left(\frac{4mx}{1-a}\right) + 8mx\,\sin\left(\frac{4mx}{1-a}\right)\right]. \tag{9.34}$$

     Note that the function indeed belongs to $\mathsf{D}(H)$ because necessarily $\frac{2m}{1-a} \in \mathbb{N}$, *i.e.* $\lambda \in \sigma_0$. Hence, the algebraic multiplicity of λ is at least three. To see that the algebraic multiplicity is not higher than three, it is enough to verify that

     $$\begin{aligned}(\phi_1, \xi) &= -\bar{A}_+ B\,\frac{\pi^2}{128m}\,(1-a)^2(1+a)\,\cos\left(m\pi\,\frac{1+a}{1-a}\right)\cos(m\pi) \neq 0\,,\\ (\phi_2, \xi) &= \bar{A}_- B\,\frac{\pi^2}{128m}\,(1-a)^2(1+a)\,\cos\left(m\pi\,\frac{1+a}{1-a}\right)\cos(m\pi) \neq 0\,.\end{aligned} \tag{9.35}$$

- $\boxed{+1 \text{ class eigenvalues}}$ Let $\lambda = \left(\frac{4m}{1+a}\right)^2$ with $m \in \mathbb{N}^*$.

  1. If $m\frac{1-a}{1+a} \notin \mathbb{N}$ (generic situation), we already know that the eigenvalue λ is geometrically simple. The functions ψ and ϕ are given by (9.15) and (9.26), respectively. Since
  $$(\phi, \psi) = \bar{A}_- B \, \frac{\pi}{4} \, (1+a) \, \sin\left(m\pi \, \frac{1-a}{1+a}\right) \cos(m\pi) \neq 0 \,, \tag{9.36}$$
  the eigenvalue λ is algebraically simple too.
  2. If $m\frac{1-a}{1+a} \in \mathbb{N}$ (exceptional situation), we already know that the eigenvalue λ has geometric multiplicity two. The two eigenfunctions ψ_1, ψ_2 of H and the two eigenfunctions ϕ_1, ϕ_2 of H^* are given by (9.16) and (9.27), respectively. Since
  $$\begin{aligned} (\phi_1, \psi_1) &= \bar{A}_+ A \, \frac{\pi}{4} \, (1-a) \, \cos\left(m\pi \, \frac{1-a}{1+a}\right) \cos(m\pi) \neq 0 \,, \\ (\phi_2, \psi_1) &= \bar{A}_- A \, \frac{\pi}{4} \, (1+a) \, \cos\left(m\pi \, \frac{1-a}{1+a}\right) \cos(m\pi) \neq 0 \,, \\ (\phi_1, \psi_2) &= 0 = (\phi_2, \psi_2) \,, \end{aligned} \tag{9.37}$$
  there might be a generalised eigenvector ξ of H associated with ψ_2. In fact, the linearly independent solution of $(H-\lambda)\xi = \psi_2$ reads
  $$\xi(x) := -B \, \frac{1+a}{64m^2} \left[(1+a) \, \cos\left(\frac{4mx}{1+a}\right) + 8mx \, \sin\left(\frac{4mx}{1+a}\right)\right] . \tag{9.38}$$
  Note that the function indeed belongs to $\mathsf{D}(H)$ because necessarily $\frac{2m}{1+a} \in \mathbb{N}$, *i.e.* $\lambda \in \sigma_0$. Hence, the algebraic multiplicity of λ is at least three. To see that the algebraic multiplicity is not higher than three, it is enough to verify that
  $$\begin{aligned} (\phi_1, \xi) &= -\bar{A}_+ B \, \frac{\pi^2}{128m} \, (1+a)^2 (1-a) \, \cos\left(m\pi \, \frac{1-a}{1+a}\right) \cos(m\pi) \neq 0 \,, \\ (\phi_2, \xi) &= \bar{A}_- B \, \frac{\pi^2}{128m} \, (1+a)^2 (1-a) \, \cos\left(m\pi \, \frac{1-a}{1+a}\right) \cos(m\pi) \neq 0 \,. \end{aligned} \tag{9.39}$$

  We remark that (9.38) can be deduced from (9.34) by the replacement $m \mapsto m\frac{1-a}{1+a}$, which reflects the relationship between the exceptional situations in the $+1$ and -1 classes.

- $\boxed{0 \text{ class eigenvalues}}$ Let $\lambda = (2m)^2$ with $m \in \mathbb{N}$.

  1. If $m = 0$, we already know that λ is geometrically simple. The functions ψ and ϕ are given by (9.18) and (9.28), respectively. Since
  $$(\phi, \psi) = -\bar{C} B \, \frac{\pi^2}{4} (1-a^2) \neq 0 \,, \tag{9.40}$$
  the zero eigenvalue is always algebraically simple.
  2. If $m \neq 0$ and $ma \notin \mathbb{N}$ (generic situation), we already know that the eigenvalue λ is geometrically simple. The functions ψ and ϕ are given by (9.19) and (9.29), respectively. Since
  $$(\phi, \psi) = \bar{C} B \, \frac{\pi}{2} \, \frac{1 - \cos(m\pi)\cos(m\pi a)}{\sin(m\pi a)} \neq 0 \,, \tag{9.41}$$
  the eigenvalue λ is algebraically simple too.
  3. If $m \neq 0$ and $ma \in \mathbb{N}$ (exceptional situation), we distinguish two cases:
     (a) If $m(1+a)$ is odd (which necessarily implies that $m(1-a)$ is odd as well), we already know that the eigenvalue λ is geometrically simple. The eigenfunction ψ of H is given by (9.20) and the corresponding eigenfunction ϕ of H^* is given by (9.29). Since
     $$(\phi, \psi) = \bar{C} A \, \frac{\pi}{2} \cos(m\pi) \neq 0 \,, \tag{9.42}$$
     the eigenvalue λ is algebraically simple too.

(b) If $m(1+a)$ is even (which necessarily implies that $m(1-a)$ is even as well), we already know that the eigenvalue λ has geometric multiplicity two. The two eigenfunctions ψ_1, ψ_2 of H and the two eigenfunctions ϕ_1, ϕ_2 of H^* are given by (9.21) and (9.30), respectively. Since

$$\begin{aligned} (\phi_1, \psi_1) &= \bar{A}_+ A \, \frac{\pi}{4} \, (1-a) \, \cos(m\pi) \neq 0 \,, \\ (\phi_2, \psi_1) &= \bar{A}_- A \, \frac{\pi}{4} \, (1+a) \, \cos(m\pi) \neq 0 \,, \\ (\phi_1, \psi_2) &= 0 = (\phi_2, \psi_2) \,, \end{aligned} \tag{9.43}$$

there might be a generalised eigenvector ξ of H associated with ψ_2. In fact, the linearly independent solution of $(H-\lambda)\xi = \psi_2$ reads

$$\xi(x) := -B \, \frac{1}{16m^2} \left[\cos(2mx) + 4mx \, \sin(2mx)\right] . \tag{9.44}$$

Hence, the algebraic multiplicity of λ is at least three. To see that the algebraic multiplicity is not higher than three, it is enough to verify that

$$\begin{aligned} (\phi_1, \xi) &= -\bar{A}_+ B \, \frac{\pi}{64m} \, (1-a^2) \, \cos(m\pi) \neq 0 \,, \\ (\phi_2, \xi) &= \bar{A}_- B \, \frac{\pi}{64m} \, (1-a^2) \, \cos(m\pi) \neq 0 \,. \end{aligned} \tag{9.45}$$

We remark that (9.44) can be deduced from (9.34) by the replacement $m \mapsto m\frac{1-a}{2}$, which reflects the relationship between the exceptional situations in the 0 and -1 classes.

We summarise the established geometric and algebraic properties of the eigenvalues of H in the following proposition.

Proposition 9.4.

1. *If $a \notin \mathbb{Q}$, then all the eigenvalues of H are algebraically simple.*
2. *Let $a \in \mathbb{Q}$. Each point of $\sigma(H) \setminus (\sigma_{-1} \cap \sigma_{+1})$ corresponds to an eigenvalue of H of algebraic multiplicity one. Each point of $\sigma_{-1} \cap \sigma_{+1} = \sigma_{-1} \cap \sigma_{+1} \cap \sigma_0$ corresponds to an eigenvalue of H of geometric multiplicity two and algebraic multiplicity three.*

Theorem 9.1 follows as a consequence of this proposition.

9.6 The resolvent

Now we turn to a study of the resolvent of H in some further detail. We have already seen in Section 9.4 that the resolvent is a compact operator (*cf* Proposition 9.3). However, the compactness by itself is not sufficient to analyse completeness of eigenfunctions and related properties. In this section we therefore give an explicit formula for the integral kernel of the resolvent and show that it is a trace-class operator.

Let us denote by H^0 the Laplacian in $\left(-\frac{\pi}{2}, \frac{\pi}{2}\right)$ with Dirichlet boundary conditions, *i.e.*,

$$H^0\psi := -\psi'' \,, \qquad \psi \in \mathsf{D}(H^0) := \left\{\psi \in H^2((-\tfrac{\pi}{2}, \tfrac{\pi}{2})) \;\middle|\; \psi(-\tfrac{\pi}{2}) = 0 = \psi(\tfrac{\pi}{2})\right\} ,$$

and by $R^0(\lambda)$ its resolvent. It is well known that $\sigma(H^0) = \{n^2\}_{n\in\mathbb{N}^*}$ and that $R^0(\lambda)$ acts as an integral operator with explicit kernel (see, *e.g.*, [10, Sec. III.2.3])

$$G^0_\lambda(x,y) := \frac{-1}{k\sin(2k\frac{\pi}{2})} \begin{cases} \sin(k(x+\frac{\pi}{2}))\sin(k(y-\frac{\pi}{2})) \,, & x<y \,, \\ \sin(k(y+\frac{\pi}{2}))\sin(k(x-\frac{\pi}{2})) \,, & x>y \,, \end{cases} \tag{9.46}$$

where $k \in \mathbb{C}$ is such that $k^2 = \lambda \in \mathbb{C} \setminus \sigma(H^0)$.

We have the following Krein-type formula for the resolvent $R(\lambda)$ of H.

Proposition 9.5. *For every $\lambda \in \mathbb{C} \setminus [\sigma(H) \cup \sigma(H^0)]$, the resolvent $R(\lambda)$ of H admits the decomposition*

$$(R(\lambda)f)(x) = (R^0(\lambda)f)(x) + \frac{h^x(\lambda)}{1 - h^{\frac{\pi}{2}a}(\lambda)} \, (R^0(\lambda)f)(\tfrac{\pi}{2}a) \,, \tag{9.47}$$

with any $f \in L^2((-\frac{\pi}{2}, \frac{\pi}{2}))$ and $x \in [-\frac{\pi}{2}, \frac{\pi}{2}]$, where

$$h^x(\lambda) := \frac{\cosh(\sqrt{-\lambda}\,x)}{\cosh(\sqrt{-\lambda}\,\frac{\pi}{2})} \,.$$

Proof. First of all, notice that $R(\lambda)$ introduced by (9.47) is a bounded operator on $L^2((-\frac{\pi}{2},\frac{\pi}{2}))$. Indeed, it is the case of $R^0(\lambda)$ for $\lambda \in \mathbb{C}\setminus\sigma(H^0)$ and the second term on the right hand side of (9.47) represents a rank-one perturbation of $R^0(\lambda)$. More specifically,

$$\frac{h^x(\lambda)}{1-h^{\frac{\pi}{2}a}(\lambda)}\,(R^0(\lambda)f)(\tfrac{\pi}{2}a) = g_1(x)\,(g_2,f)\,,$$

where

$$g_1(x) := \frac{h^x(\lambda)}{1-h^{\frac{\pi}{2}a}(\lambda)} \qquad \text{and} \qquad g_2(y) := \overline{G^0_\lambda(\tfrac{\pi}{2}a,y)}$$

are continuous functions on $[-\frac{\pi}{2},\frac{\pi}{2}]$ for all $\lambda \in \mathbb{C}\setminus[\sigma(H)\cup\sigma(H^0)]$. Next, we observe that the function $x \mapsto (R(\lambda)f)(x)$ solves the boundary conditions

$$(R(\lambda)f)(-\tfrac{\pi}{2}) = (R(\lambda)f)(\tfrac{\pi}{2}a) = (R(\lambda)f)(\tfrac{\pi}{2})\,.$$

Indeed,

$$(R(\lambda)f)(-\tfrac{\pi}{2}) = \frac{1}{1-h^{\frac{\pi}{2}a}(\lambda)}\,(R^0(\lambda)f)(\tfrac{\pi}{2}a) = (R(\lambda)f)(\tfrac{\pi}{2})$$

and

$$(R(\lambda)f)(\tfrac{\pi}{2}a) = (R^0(\lambda)f)(\tfrac{\pi}{2}a)\left(1+\frac{h^{\frac{\pi}{2}a}(\lambda)}{1-h^{\frac{\pi}{2}a}(\lambda)}\right) = \frac{1}{1-h^{\frac{\pi}{2}a}(\lambda)}\,(R^0(\lambda)f)(\tfrac{\pi}{2}a)\,.$$

Furthermore, it is straightforward to check that, for every $f \in L^2((-\frac{\pi}{2},\frac{\pi}{2}))$, $R(\lambda)f \in H^2((-\frac{\pi}{2},\frac{\pi}{2}))$ and

$$-(R(\lambda)f)'' - \lambda\,(R(\lambda)f) = f\,.$$

Hence, $R(\lambda) : L^2((-\frac{\pi}{2},\frac{\pi}{2})) \to \mathsf{D}(H)$ and $R(\lambda)$ is the right inverse of $H-\lambda$. To show that $R(\lambda)$ is also the left inverse of $H-\lambda$, one can employ (9.46), which in particular yields the useful identity

$$[R^0(\lambda)(H-\lambda)\psi](x) = \psi(x) - \frac{\cos(kx)}{\cos(k\frac{\pi}{2})}\,\psi(\tfrac{\pi}{2}a)$$

for every $\psi \in \mathsf{D}(H)$ and $k \in \mathbb{C}$ such that $k^2 = \lambda \in \mathbb{C}\setminus\sigma(H^0)$. ☐

Remark 9.1. Formula (9.47) can be deduced from [8, Thm. 1] (see also [8, Eq. (3.5)]). However, since the transition semigroup of [8] is defined on a different functional space, the present proof of Proposition 9.5 is still needed.

From Proposition 9.5 we get the following corollary.

Proposition 9.6. *For every $\lambda \in \mathbb{C}\setminus\sigma(H)$, the resolvent $R(\lambda)$ is a trace-class operator.*

Proof. From Proposition 9.5 we see that the resolvent $R(\lambda)$ is a rank-one perturbation of $R^0(\lambda)$. Since $R^0(\lambda)$ is well known to be trace-class, rank-one operators are obviously trace-class and trace-class operators form a two-sided ideal in the space of bounded operators (see, *e.g.*, [18, Thm. 7.8]), we immediately obtain the claim from Proposition 9.5 for every $\lambda \in \mathbb{C}\setminus[\sigma(H)\cup\sigma(H^0)]$. By the first resolvent identity [18, Thm. 5.13] and the two-sided ideal properties of trace-class operators, the trace-class property then easily extends to all λ in the resolvent set of H. ☐

9.7 Basis properties

Since the spectrum of H is real, it is natural to ask whether H is similar to a self-adjoint operator. This question is related to basis properties of the eigenfunctions of H.

9.7.1 Completeness

Recall that the *completeness* of a family of vectors $\{\psi_j\}_{j\in\mathbb{N}}$ in a Hilbert space $\mathcal{H}$ means that its span is dense in $\mathcal{H}$, or equivalently, $(\{\psi_j\}_{j\in\mathbb{N}})^\perp = \{0\}$.

Theorem 9.4. *The eigenfunctions of H together with the generalised eigenfunctions form a complete set in $L^2((-\frac{\pi}{2},\frac{\pi}{2}))$.*

Proof. The m-accretivity of $\tilde{H} := H + \frac{1}{16}$ implies $\Re(\psi, \tilde{H}\psi) \geq 0$ for all $\psi \in \mathsf{D}(H)$. Consequently, $-i\tilde{H}$ is dissipative, *i.e.* $\Im\langle\psi, -i\tilde{H}\psi\rangle \leq 0$ for all $\psi \in \mathsf{D}(H)$. It is then easy to check that the imaginary part of the resolvent of $-i\tilde{H}$ at $z < 0$ is non-negative, *i.e.*,

$$\frac{1}{2i}\left((-i\tilde{H} - z)^{-1} - (i\tilde{H}^* - z)^{-1}\right) \geq 0 \tag{9.48}$$

in the sense of forms. Note that the resolvent of $-i\tilde{H}$ is well defined for all non-imaginary points, because the spectrum of H is real. By virtue of Proposition 9.6, $(H+1)^{-1}$ and thus also $(-i\tilde{H} - z)^{-1}$ are trace-class operators. Combining this fact with (9.48), it is enough to apply the completeness theorem [7, Thm. VII.8.1] to the resolvent operator $(-i\tilde{H} - z)^{-1}$. ☐

As a consequence of this theorem and Proposition 9.4, we get

Corollary 9.1. *If $a \notin \mathbb{Q}$, the eigenfunctions of H form a complete set in $L^2((-\frac{\pi}{2}, \frac{\pi}{2}))$.*

Since the quasi-m-accretivity of H implies the same property for H^* and the spectrum is real, the proofs of the results of Theorem 9.4 and Corollary 9.1 apply to the eigensystem of H^* as well.

9.7.2 Minimal completeness

We say that a complete set of vectors $\{\psi_j\}_{j\in\mathbb{N}}$ in a Hilbert space $\mathcal{H}$ is *minimal complete* if the removal of any term makes it incomplete. By [5, Prob. 3.3.2], $\{\psi_j\}_{j\in\mathbb{N}}$ is minimal complete if, and only if, there exists a sequence $\{\phi_j\}_{j\in\mathbb{N}} \subset \mathcal{H}$ such that the pair is *biorthogonal*, *i.e.*,

$$(\phi_j, \psi_k) = \delta_{jk} \tag{9.49}$$

for all $j, k \in \mathbb{N}$.

In our case, we form $\{\psi_j\}_{j\in\mathbb{N}}$ from the eigenfunctions ψ of H together with the generalised eigenfunctions ξ. The dual sequence $\{\phi_j\}_{j\in\mathbb{N}}$ will be then given by the eigenfunctions ϕ of H^* together with its generalised eigenfunctions η that we determine only now.

- $\boxed{-1\text{ class eigenvalues}}$ Let $\lambda = \left(\frac{4m}{1-a}\right)^2$ with $m \in \mathbb{N}^*$.

  1. If $m\frac{1+a}{1-a} \notin \mathbb{N}$ (generic situation), the eigenvalue λ is algebraically simple. In view of (9.32), the functions ψ and ϕ given by (9.13) and (9.24), respectively, can be normalised in such a way that (9.49) holds.
  2. If $m\frac{1+a}{1-a} \in \mathbb{N}$ (exceptional situation), the eigenvalue λ has geometric multiplicity two and algebraic multiplicity three. In view of (9.33) and (9.35), the functions ψ_1, ξ given by (9.14) and (9.34) and the functions ϕ_1, ϕ_2 given by (9.25) are mutually biorthogonal when normalised properly. We still need to find the function dual to ψ_2 from (9.14). To this aim, we consider the equation $(H^* - \lambda)\eta = \phi_1 + \phi_2$ and find the linearly independent solution

  $$\eta(x) := \begin{pmatrix} A_- \frac{1-a}{64m^2}\left[8m(x+\frac{\pi}{2})\cos\left(\frac{4m}{1-a}(x+\frac{\pi}{2})\right) - (1-a)\sin\left(\frac{4m}{1-a}(x+\frac{\pi}{2})\right)\right] \\ A_+ \frac{1-a}{64m^2}\left[8m(x-\frac{\pi}{2})\cos\left(\frac{4m}{1-a}(x-\frac{\pi}{2})\right) - (1-a)\sin\left(\frac{4m}{1-a}(x-\frac{\pi}{2})\right)\right] \end{pmatrix}, \tag{9.50}$$

  which indeed belongs to $\mathsf{D}(H^*)$ provided that

  $$A_-(1+a) = -A_+(1-a), \tag{9.51}$$

  where $A_\pm$ are the normalisation constants from (9.25). Since

  $$(\eta, \psi_2) = \bar{A}_- B \frac{\pi^2}{64m}(1-a)(1+a)\cos\left(m\pi\frac{1+a}{1-a}\right)\cos(m\pi) \neq 0, \tag{9.52}$$

  we can eventually choose the normalisation constants in such a way that ψ_2 and η is the remaining biorthogonal pair.

- $\boxed{+1\text{ class eigenvalues}}$ Let $\lambda = \left(\frac{4m}{1+a}\right)^2$ with $m \in \mathbb{N}^*$.

  1. If $m\frac{1-a}{1+a} \notin \mathbb{N}$ (generic situation), the eigenvalue λ is algebraically simple. In view of (9.36), the functions ψ and ϕ given by (9.15) and (9.26), respectively, can be normalised in such a way that (9.49) holds.

2. If $m\frac{1-a}{1+a} \in \mathbb{N}$ (exceptional situation), then λ belongs to the exceptional situation in the -1 class too. Hence, the analysis is reduced to the preceding case. In particular, the formula (9.50) holds here after the replacement $m \mapsto m\frac{1-a}{1+a}$.

- $\boxed{\text{0 class eigenvalues}}$ Let $\lambda = (2m)^2$ with $m \in \mathbb{N}$.

1. If $m = 0$, the eigenvalue λ is algebraically simple. In view of (9.40), the functions ψ and ϕ given by (9.18) and (9.28), respectively, can be normalised in such a way that (9.49) holds.
2. If $m \neq 0$ and $ma \notin \mathbb{N}$ (generic situation), the eigenvalue λ is algebraically simple. The functions ψ and ϕ given by (9.19) and (9.29), respectively, can be normalised in such a way that (9.49) holds.
3. If $m \neq 0$ and $ma \in \mathbb{N}$ (exceptional situation), we distinguish two cases:
   (a) If $m(1+a)$ is odd (which necessarily implies that $m(1-a)$ is odd as well), the eigenvalue λ is algebraically simple. In view of (9.42), the functions ψ and ϕ given by (9.20) and (9.29), respectively, can be normalised in such a way that (9.49) holds.
   (b) If $m(1+a)$ is even (which necessarily implies that $m(1-a)$ is even as well), then λ belongs to the exceptional situation in the -1 class too. In particular, the formula (9.50) holds here after the replacement $m \mapsto m\frac{1-a}{2}$.

We summarise the results of this subsection in the following theorem.

Theorem 9.5. *The eigenfunctions of H together with the generalised eigenfunctions form a mutually biorthogonal pair in $L^2((-\frac{\pi}{2}, \frac{\pi}{2}))$. Consequently, the eigenfunctions of H together with the generalised eigenfunctions form a minimal complete set in $L^2((-\frac{\pi}{2}, \frac{\pi}{2}))$. In particular, the eigenfunctions of H form a minimal complete set in $L^2((-\frac{\pi}{2}, \frac{\pi}{2}))$ if, and only if, $a \notin \mathbb{Q}$.*

An analogue of this theorem holds for the adjoint operator H^* as well.

9.7.3 Conditional basis

Recall that $\{\psi_j\}_{j\in\mathbb{N}} \subset \mathcal{H}$ is a *conditional (or Schauder) basis* in a Hilbert space $\mathcal{H}$ if every $f \in \mathcal{H}$ has a unique expansion in the vectors $\{\psi_j\}_{j\in\mathbb{N}}$, *i.e.*,

$$\forall f \in \mathcal{H}, \quad \exists! \{\alpha_j\}_{j\in\mathbb{N}} \subset \mathbb{C}, \quad f = \sum_{j=0}^{\infty} \alpha_j \psi_j \,. \tag{9.53}$$

The minimal completeness of $\{\psi_j\}_{j\in\mathbb{N}}$ is a necessary condition for $\{\psi_j\}_{j\in\mathbb{N}}$ to be a conditional basis. By [5, Lem. 3.3.3] (see also [14, Prop. 5]), another necessary condition for $\{\psi_j\}_{j\in\mathbb{N}}$ being a conditional basis is that the norms of the one-dimensional projections

$$P_j := \psi_j(\phi_j, \cdot) \tag{9.54}$$

are uniformly bounded in j. Since $\|P_j\| = \|\psi_j\|\|\phi_j\|$, this check reduces to a computation of elementary trigonometric integrals in our case.

- $\boxed{-1 \text{ class eigenvalues}}$ Let $\lambda = \left(\frac{4m}{1-a}\right)^2$ with $m \in \mathbb{N}^*$.

1. If $m\frac{1+a}{1-a} \notin \mathbb{N}$ (generic situation), recalling (9.13), (9.24) and (9.32), we define $P := \psi(\phi, \cdot)$ and find

$$\|P\| = \frac{\sqrt{\frac{1}{8}\left[4\pi + \frac{1-a}{m}\sin\left(\frac{4m\pi}{1-a}\right)\right]}}{\sqrt{\frac{\pi}{4}(1-a)}\left|\sin\left(m\pi\frac{1+a}{1-a}\right)\right|} \,. \tag{9.55}$$

2. If $m\frac{1+a}{1-a} \in \mathbb{N}$ (exceptional situation), recalling (9.14), (9.25), (9.34), (9.50), (9.33), (9.35) and (9.52), we define $P_1 := \psi_1(\phi_1, \cdot)$, $P_2 := \psi_2(\eta, \cdot)$, $P_3 := \xi(\phi_2, \cdot)$, and find

$$\begin{aligned} \|P_1\| &= \frac{\sqrt{2}}{\sqrt{1-a}} \,, \\ \|P_2\| &= \frac{\sqrt{15(1-a) + 16m^2\pi^2(1+a)}}{2\sqrt{3}\,\pi\sqrt{1+a}\,m} \,, \\ \|P_3\| &= \frac{\sqrt{64m^2\pi^2 - 36(1-a)^2}}{2\sqrt{6}\,\pi\sqrt{1+a}\,(1-a)\,m} \,. \end{aligned} \tag{9.56}$$

- $\boxed{+1 \text{ class eigenvalues}}$ Let $\lambda = \left(\frac{4m}{1+a}\right)^2$ with $m \in \mathbb{N}^*$.

  1. If $m\frac{1-a}{1+a} \notin \mathbb{N}$ (generic situation), recalling (9.15), (9.26) and (9.36), we define $P := \psi(\phi, \cdot)$ and find

$$\|P\| = \frac{\sqrt{\frac{1}{8}\left[4\pi + \frac{1+a}{m}\sin\left(\frac{4m\pi}{1+a}\right)\right]}}{\sqrt{\frac{\pi}{4}(1+a)}\left|\sin\left(m\pi\frac{1-a}{1+a}\right)\right|}\,. \tag{9.57}$$

  2. If $m\frac{1-a}{1+a} \in \mathbb{N}$ (exceptional situation), then λ belongs to the exceptional situation in the -1 class too. Hence, the analysis is reduced to the preceding case.

- $\boxed{0 \text{ class eigenvalues}}$ Let $\lambda = (2m)^2$ with $m \in \mathbb{N}$.

  1. If $m = 0$, recalling (9.18), (9.28) and (9.40), we define $P := \psi(\phi, \cdot)$ and find

$$\|P\| = \sqrt{\frac{4}{3}}\,. \tag{9.58}$$

  2. If $m \neq 0$ and $ma \notin \mathbb{N}$ (generic situation), recalling (9.19), (9.29) and (9.41), we define $P := \psi(\phi, \cdot)$ and find

$$\|P\| = \frac{\sqrt{2}}{\sqrt{1 - \cos\big(m\pi(1+a)\big)}}\,. \tag{9.59}$$

  3. If $m \neq 0$ and $ma \in \mathbb{N}$ (exceptional situation), we distinguish two cases:

     (a) If $m(1+a)$ is odd (which necessarily implies that $m(1-a)$ is odd as well), recalling (9.20), (9.29) and (9.42), we define $P := \psi(\phi, \cdot)$ and find

$$\|P\| = 1\,. \tag{9.60}$$

     (b) If $m(1+a)$ is even (which necessarily implies that $m(1-a)$ is even as well), then λ belongs to the exceptional situation in the -1 class too. Hence, the analysis is reduced to the case studied above.

Now we are in a position to establish Theorem 9.2 announced in the introduction.

Proof of Theorem 9.2. If $a \in \mathbb{Q}$, the eigenfunctions of H cannot form a conditional basis in $L^2((-\frac{\pi}{2}, \frac{\pi}{2}))$, because they are not even minimal complete by Theorem 9.5. To disprove the basis property in the case $a \notin \mathbb{Q}$, we show that the spectral projections (9.54) are not uniformly bounded. To this aim, we consider for instance (9.59). By Dirichlet's theorem on Diophantine approximation of irrational numbers (see, *e.g.*, [17, Thm. 1A]), there exist sequences of integers $(p_k, q_k) \in \mathbb{Z} \times \mathbb{N}^*$ such that $|p_k| \to \infty$ and $q_k \to \infty$ as $k \to \infty$ and

$$\left|a - \frac{p_k}{q_k}\right| < \frac{1}{q_k^2}$$

for every $k \in \mathbb{N}$. Consequently, choosing $m := 2q_k$, we get

$$\cos\big(m\pi(1+a)\big) = \cos\left(2q_k\pi\left(a - \frac{p_k}{q_k}\right)\right) \xrightarrow[k\to\infty]{} 1\,.$$

Restricting to spectral projections (9.59) from the 0 class, we thus obtain

$$\sup_{j\in\mathbb{N}} \|P_j\| \geq \sup_{m\in\mathbb{N}^*} \frac{\sqrt{2}}{\sqrt{1 - \cos\big(m\pi(1+a)\big)}} \geq \sup_{k\in\mathbb{N}^*} \frac{\sqrt{2}}{\sqrt{1 - \cos\big(2q_k\pi(1+a)\big)}} = \infty\,.$$

This concludes the proof of the theorem. □

Remark 9.2. If $a \in \mathbb{Q}$, it is still possible that the generalised eigensystem (*i.e.* the collection of eigenfunctions and generalised eigenfunctions) is a conditional basis. We leave this question open here. Anyway, let us demonstrate that the projections (9.54), where $\{\psi_j\}_{j\in\mathbb{N}}$ and $\{\phi_j\}_{j\in\mathbb{N}}$ denote the biorthogonal pair formed by the eigenfunctions and generalised eigenfunctions of H and H^*, respectively, are uniformly bounded. The formulae (9.56), (9.58) and (9.60) are obviously uniformly bounded in $m \in \mathbb{N}^*$. To show that it is the case for the remaining norms of one-dimensional projections (9.55), (9.57) and (9.59), too, it is enough to write $a = \frac{p}{q}$ with some integers $(p,q) \in \mathbb{Z} \times \mathbb{Z}^*$ (since $|a| < 1$, we have $|q| > |p|$) and use the elementary estimates

$$\begin{aligned}
\left|\sin\left(m_{-1}\pi\frac{1+a}{1-a}\right)\right| &\geq \frac{2}{\pi}\,\operatorname{dist}\left(m_{-1}\pi\frac{1+a}{1-a}, \pi\mathbb{Z}\right) \geq \frac{2}{|q-p|}\,, \\
\left|\sin\left(m_{+1}\pi\frac{1-a}{1+a}\right)\right| &\geq \frac{2}{\pi}\,\operatorname{dist}\left(m_{+1}\pi\frac{1-a}{1+a}, \pi n\right) \geq \frac{2}{|q+p|}\,, \\
1-\cos\big(m_0\pi(1+a)\big) &\geq \frac{4}{\pi^2}\,\operatorname{dist}\Big(m_0\pi(1+a), 2\pi\mathbb{Z}\Big)^2 \geq \frac{4}{q^2}\,,
\end{aligned}$$

valid for all $m_{-1}, m_{+1}, m_0 \in \mathbb{N}^*$ such that $m_{\pm 1}\frac{1\mp a}{1\pm a} \notin \mathbb{N}$ and $m_0 a \notin \mathbb{N}$.

9.7.4 Metric operator

We finally recall that $\{\psi_j\}_{j\in\mathbb{N}}$, normalised to 1 in a Hilbert space $\mathcal{H}$, is an *unconditional (or Riesz) basis* if it is a conditional basis and the inequality

$$\forall f \in \mathcal{H}, \qquad C^{-1}\|f\|^2 \leq \sum_{j=0}^{\infty} |(\psi_j, f)|^2 \leq C\|f\|^2 \tag{9.61}$$

holds with a positive constant C independent of f. If $\{\psi_j\}_{j\in\mathbb{N}}$ is a normalised set of eigenfunctions of an operator H with compact resolvent in $\mathcal{H}$, then H is similar to a normal operator via bounded and boundedly invertible transformation if, and only if, $\{\psi_j\}_{j\in\mathbb{N}}$ is an unconditional basis in $\mathcal{H}$, *cf* [5, Thm. 3.4.5]. The latter is equivalent to the similarity to a self-adjoint operator if the spectrum of H is in addition real.

The similarity to a self-adjoint operator is also equivalent to the existence of a *metric operator*, *i.e.* a positive, bounded and boundedly invertible operator Θ such that (9.3) holds (*cf* [13, Prop. 5.5.2]). The metric operator can be constructed by the formula

$$\Theta = \sum_{j=0}^{\infty} \phi_j(\phi_j, \cdot)\,, \tag{9.62}$$

where ϕ_j are eigenfunctions of H^*.

In our case, H cannot be similar to a self-adjoint operator via bounded and boundedly invertible transformation because the eigenfunctions of H do not form already a conditional basis (they are not even complete if $a \in \mathbb{Q}$), *cf* Theorem 9.2. Nonetheless, if $a \notin \mathbb{Q}$, we shall show that the relation (9.3) still holds with a positive and bounded Θ whose inverse exists but it is unbounded. Furthermore, we shall derive a closed formula for the metric operator (9.62).

Our approach is based on the following peculiar properties of the eigenbasis of H^*. Hereafter we assume $a \notin \mathbb{Q}$.

- Eigenfunctions in the -1 class are all those eigenfunctions of the Dirichlet Laplacian in $(\frac{\pi}{2}a, \frac{\pi}{2})$ which are antisymmetric with respect to the middle point $\frac{\pi}{4}(1+a)$. Putting $A_+ := \sqrt{2/[\pi(1-a)]}$, the eigenfunctions become normalised to 1 in $L^2((\frac{\pi}{2}a, \frac{\pi}{2}))$. Consequently,
$$\sum_{\lambda_j\in\sigma_-} \phi_j(\phi_j, \cdot) = 0 \oplus P_+\,,$$
where P_+ is the antisymmetric projection
$$(P_+ f)(x) := \frac{f(x) - f(-x + \frac{\pi}{2}(1+a))}{2}\,, \qquad x \in [\tfrac{\pi}{2}a, \tfrac{\pi}{2}]\,.$$
The direct sum is again with respect to the decomposition $L^2((-\frac{\pi}{2}, \frac{\pi}{2}a)) \oplus L^2((\frac{\pi}{2}a, \frac{\pi}{2}))$.
- Eigenfunctions in the $+1$ class are all those eigenfunctions of the Dirichlet Laplacian in $(-\frac{\pi}{2}, \frac{\pi}{2}a)$ which are antisymmetric with respect to the middle point $-\frac{\pi}{4}(1-a)$. Putting $A_- := \sqrt{2/[\pi(1+a)]}$, the eigenfunctions become normalised to 1 in $L^2((-\frac{\pi}{2}, \frac{\pi}{2}a))$. Consequently,
$$\sum_{\lambda_j\in\sigma_+} \phi_j(\phi_j, \cdot) = P_- \oplus 0\,,$$
where P_- is the antisymmetric projection
$$(P_- f)(x) := \frac{f(x) - f(-x - \frac{\pi}{2}(1-a))}{2}\,, \qquad x \in [-\tfrac{\pi}{2}, \tfrac{\pi}{2}a]\,.$$

- Eigenfunctions in the 0 class except for (9.28) are all those eigenfunctions of the Dirichlet Laplacian in $(-\frac{\pi}{2},\frac{\pi}{2})$ which are antisymmetric with respect to the middle point 0. Putting $C := \sqrt{2/\pi}$, the eigenfunctions become normalised to 1 in $L^2((-\frac{\pi}{2},\frac{\pi}{2}))$. Consequently,

$$\sum_{\lambda_j\in\sigma_0\setminus\{0\}} \phi_j(\phi_j,\cdot) = P_0\,,$$

where P_0 is the antisymmetric projection

$$(P_0 f)(x) := \frac{f(x)-f(-x)}{2}\,, \qquad x\in[-\tfrac{\pi}{2},\tfrac{\pi}{2}]\,.$$

- Finally, let us denote the eigenfunction (9.28) corresponding to the zero eigenvalue by ϕ_0 and let us put the normalisation constant C equal to one for instance. Then we get a rank-one operator

$$\sum_{\lambda_j=0} \phi_j(\phi_j,\cdot) = \phi_0(\phi_0,\cdot)\,.$$

Summing up, we arrive at the following particularly simple form for the metric operator defined by (9.62)

$$\Theta = \phi_0(\phi_0,\cdot) + P_0 + P_-\oplus P_+\,. \tag{9.63}$$

Let us carefully verify all the required properties of the metric operator, giving thus a proof Theorem 9.3 announced in the introduction.

Proof of Theorem 9.3.

- Obviously, Θ defined by (9.63) is **bounded**.
- It is **positive** just because

$$(f,\Theta f) = |(\phi_0,f)|^2 + \|P_0 f\|^2 + \|P_- f\oplus P_+ f\|^2 \geq 0 \tag{9.64}$$

for every $f\in L^2((-\frac{\pi}{2},\frac{\pi}{2}))$.

- To prove that Θ is **invertible** (*i.e.* 0 is not an eigenvalue of Θ), we need the following fact.

Lemma 9.1. *Let $a\notin\mathbb{Q}$. If $P_0 f = 0$ and $P_- f\oplus P_+ f = 0$ for some $f\in L^2((-\frac{\pi}{2},\frac{\pi}{2}))$, then $f(x)$ is a constant for almost every $x\in(-\frac{\pi}{2},\frac{\pi}{2})$.*

Proof. We decompose f into the eigenbasis of the Neumann Laplacian in $(-\frac{\pi}{2},\frac{\pi}{2})$, *i.e.*, we write

$$f = \sum_{n=0}^{\infty} \alpha_n\chi_n\,, \qquad \chi_n(x) := \begin{cases} \sqrt{\frac{2}{\pi}}\cos(nx) & \text{if} \quad n\geq 1 \text{ is even}\,,\\ \sqrt{\frac{2}{\pi}}\sin(nx) & \text{if} \quad n\geq 1 \text{ is odd}\,,\\ \sqrt{\frac{1}{\pi}} & \text{if} \quad n=0\,, \end{cases}$$

where $\alpha_n := (\chi_n, f)$. Requiring $P_0 f = 0$ immediately yields that the coefficients α_n vanish for all odd n. At the same time, an explicit computation gives

$$(\chi_m, P_-\chi_n\oplus P_+\chi_n) = \frac{1}{2}\left[1-\cos(\frac{n\pi}{2})\cos(\frac{n\pi a}{2})\right]\delta_{mn}$$

for all even m,n. Summing up,

$$\|P_0 f\|^2 + \|P_- f\oplus P_+ f\|^2 = \sum_{n \text{ odd}} |\alpha_n|^2 + \sum_{n \text{ even}} |\alpha_n|^2 \frac{1}{2}\left[1-\cos(\frac{n\pi}{2})\cos(\frac{n\pi a}{2})\right]\,.$$

If $a\notin\mathbb{Q}$, the square bracket is positive for all $n\neq 0$ and we may conclude that $\alpha_n = 0$ for all $n\geq 1$. Consequently, $f(x) = \alpha_0\chi_0(x)$ for almost every $x\in(-\frac{\pi}{2},\frac{\pi}{2})$. □

Using this lemma, assuming that $f\neq 0$ is an eigenfunction of Θ corresponding to its zero eigenvalue, we conclude from (9.64) that $f(x) = \text{const}\in\mathbb{C}$ for almost every $x\in(-\frac{\pi}{2},\frac{\pi}{2})$ and

$$0 = (\phi_0,\psi) = \text{const}\left(\frac{\pi}{2}\right)^2 (a^2-1)\,,$$

which can be satisfied only if const $= 0$, a contradiction. Hence Θ is invertible.

- Recall that Θ is **not boundedly invertible** (*i.e.* 0 is in the continuous spectrum of Θ), otherwise the eigenfunctions of H would form an unconditional basis, which contradicts Theorem 9.2.
- Finally, let us show that the **quasi-self-adjointness** relation (9.3) holds.

  First of all, we have to check that Θ properly maps $\mathsf{D}(H)$ to $\mathsf{D}(H^*)$. It is obvious for the first term $\phi_0(\phi_0,\cdot)$ in (9.63). Let $\psi \in \mathsf{D}(H)$. We clearly have
  $$P_0 H^2((-\tfrac{\pi}{2},\tfrac{\pi}{2})) = H^2((-\tfrac{\pi}{2},\tfrac{\pi}{2}))\,, \qquad (P_- \oplus P_+)H^2((-\tfrac{\pi}{2},\tfrac{\pi}{2})) = H^2((-\tfrac{\pi}{2},\tfrac{\pi}{2}a)) \oplus H^2((\tfrac{\pi}{2}a,\tfrac{\pi}{2}))\,.$$
  Using the antisymmetric nature of the projections P_0, $P_\pm$ and the boundary conditions $f \in \mathsf{D}(H)$ satisfies, we easily find
  $$(P_-f)(-\tfrac{\pi}{2}) = 0\,, \qquad (P_+f)(\tfrac{\pi}{2}) = 0\,, \qquad (P_0f)(\pm\tfrac{\pi}{2}) = 0\,,$$
  $$(P_-f)(\tfrac{\pi}{2}a-) = 0\,, \qquad (P_+f)(\tfrac{\pi}{2}a+) = 0\,, \qquad (P_0f)(\tfrac{\pi}{2}a\pm) = \frac{f(\tfrac{\pi}{2}a-) - f(-\tfrac{\pi}{2}a)}{2}\,,$$
  and
  $$\begin{aligned} (P_0f)'(\tfrac{\pi}{2}) - (P_0f)'(-\tfrac{\pi}{2}) &= 0\,, \\ (P_0f)'(\tfrac{\pi}{2}a+) - (P_0f)'(\tfrac{\pi}{2}a-) &= 0\,, \\ (P_-f \oplus P_+f)'(\tfrac{\pi}{2}) - (P_-f \oplus P_+f)'(-\tfrac{\pi}{2}) &= \frac{f'(\tfrac{\pi}{2}) - f'(-\tfrac{\pi}{2})}{2}\,, \\ (P_-f \oplus P_+f)'(\tfrac{\pi}{2}a+) - (P_-f \oplus P_+f)'(\tfrac{\pi}{2}a-) &= \frac{f'(\tfrac{\pi}{2}) - f'(-\tfrac{\pi}{2})}{2}\,. \end{aligned}$$
  Hence $\Theta f \in \mathsf{D}(H^*)$.

  Verifying the identity $(f\psi)''(x) = (\Theta f'')(x)$ for $x \in (-\tfrac{\pi}{2},\tfrac{\pi}{2}a) \cup (\tfrac{\pi}{2}a,\tfrac{\pi}{2})$ is straightforward.

This concludes the proof of Theorem 9.3. □

9.8 Some open problems

Let us conclude this paper by suggesting some further research questions related to problems of the type (9.2). The list is certainly not complete and we just added those questions which are most directly connected with our present contribution.

- If $a \in \mathbb{Q}$, do the eigenfunctions together with the generalised eigenfunctions form a conditional basis (*cf* Remark 9.2)?
- Is there a direct operator-theoretic argument for the fact that the spectrum of the operator associated with (9.2) is always real? This has been shown in [16] using results about the zero set of trigonometric series.
- Is it possible to derive related results about the spectrum and the multiplicity for more general jump distributions than those considered in the present work?
- If one replaces the operator $-\frac{d^2}{dx^2}$ by $-\frac{\sigma^2}{2}\frac{d^2}{dx^2} - b\frac{d}{dx}$ in $(-\tfrac{\pi}{2},\tfrac{\pi}{2})$, then it is shown probabilistically partially in [12] and fully in [1] that the spectral gap, denoted by $\gamma_1(\sigma,b)$, of the corresponding diffusion with jump distribution δ_0 is given by
  $$\gamma_1(\sigma,b) = \min\left\{\lambda_0^{(0,\frac{\pi}{2})}(\sigma,b), \lambda_0^{(0,\frac{\pi}{4})}(\sigma,0)\right\}.$$
  Here we denote by $\lambda_0^{(0,l)}(\sigma,b)$ the smallest Dirichlet eigenvalue of $-\frac{\sigma^2}{2}\frac{d^2}{dx^2} - b\frac{d}{dx}$ in the interval $(0,l)$. Thus
  $$\gamma_1(\sigma,\mu) = \begin{cases} 2\sigma^2 + \frac{b^2}{2\sigma^2} & \text{if } \ |b| \le 2\sqrt{3}\,\sigma^2\,, \\ 8\sigma^2 & \text{otherwise}\,. \end{cases}$$
  In particular, the spectral gap stays constant once $|b|$ is greater than $2\sqrt{3}\sigma^2$. An investigation of the full spectrum including multiplicities and its dependence on the drift b might reveal further interesting properties.

Finally, let us mention that the stochastic process described in (9.2) is still not fully understood probabilistically; for recent developments we refer to [2].

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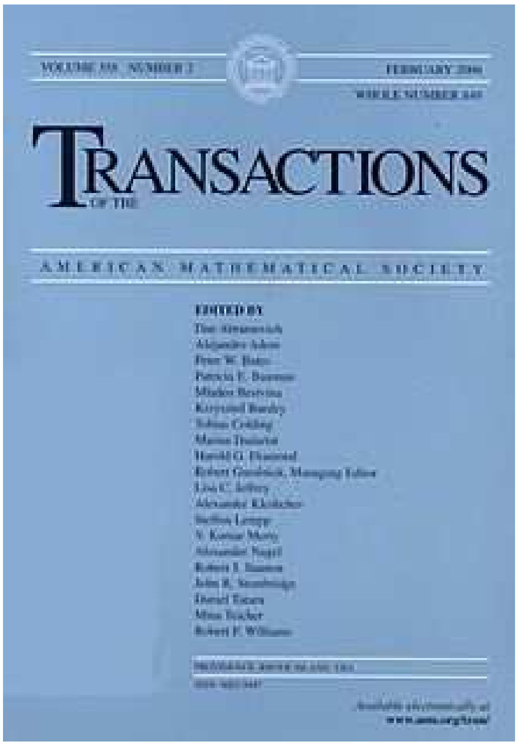
Chapter 10

Non-self-adjoint graphs



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Non-self-adjoint graphs

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Abstract. On finite metric graphs we consider Laplace operators, subject to various classes of non-self-adjoint boundary conditions imposed at graph vertices. We investigate spectral properties, existence of a Riesz basis of projectors and similarity transforms to self-adjoint Laplacians. Among other things, we describe a simple way how to relate the similarity transforms between Laplacians on certain graphs with elementary similarity transforms between matrices defining the boundary conditions.

10.1 Introduction

The subject of differential operators on metric graphs has attracted a lot of attention in the last decades. This topic has become popular under the name "quantum graphs", referring to its background and applications in quantum mechanics. Since a quantum system is described by a unitary time evolution, most of the literature has been concerned with *self-adjoint* Schrödinger operators. For more details and many references, we refer to the surveys [9, Chap. 17] and [6] together with the articles [33, 34, 35].

In other areas of physics, where a system is described by non-conservative equations of motion, it is necessary to deal with *non-self-adjoint* operators. As an example, let us mention stochastic processes on metric graphs [26, 27, 28]. Furthermore, there have been recent attempts to develop "quasi-Hermitian quantum mechanics", where physical observables are represented by non-self-adjoint operators T satisfying the *quasi-self-adjointness* relation

$$T^* = \Theta T \Theta^{-1} \tag{10.1}$$

with a bounded, boundedly invertible and positive operator $\Theta = G^*G$. The idea goes back to the paper [43] by nuclear physicists, where Θ is called *metric*, since it defines a new inner product in the underlying Hilbert space with respect to which T becomes self-adjoint. In other words, T is similar to a self-adjoint operator via the similarity transformation G, namely GTG^{-1} is self-adjoint. A consistent quantum theory can be built for quasi-self-adjoint operators.

It is not easy to decide whether a given non-self-adjoint operator is quantum-mechanically admissible, *i.e.* quasi-self-adjoint. A necessary condition for the quasi-self-adjointness of T is that its spectrum $\sigma(T)$ is real. It was noticed that many operators commuting with an anti-unitary operator called *symmetry* have the real spectrum. This observation is behind the boom of the so-called "$\mathcal{PT}$-symmetric quantum mechanics" [5, 40], which we use here as a source of interesting quasi-self-adjoint models. In this context, non-self-adjoint operators on metric graphs were previously considered in [4, 45].

The present work is motivated by the growing interest in spectral theory on network structures and by the fresh relevance of non-self-adjoint operators in quantum mechanics. We regard metric graphs as an intermediate step between Sturm-Liouville operators on intervals and partial differential operators. Indeed, we shall be able to rigorously investigate some non-trivial properties related to the spectrum and quasi-self-adjointness that one can hardly expect to obtain in such a generality in higher dimensions.

We restrict ourselves to a simple differential operator on the graph – namely the Laplacian – but consider arbitrary non-self-adjoint interface or boundary conditions on the graph vertices. The standard material about Laplacians on metric graphs is collected in the forthcoming Section 10.2. In a long Section 10.3 divided into many subsections we introduce various classes of boundary conditions for the Laplacian. The emphasis is not put on a systematic classification of non-self-adjoint boundary conditions, but rather on a diversity motivated by different applications and on intriguing examples with wild spectra.

Spectral theory for the Laplacians is developed in Section 10.4. There we also present an explicit integral-type formula for the resolvent, with a proof postponed to Appendix 10.7. In Section 10.5, we apply an abstract result of Agranovich [1] to show that the eigensystem of a non-self-adjoint Laplacian on a compact metric graph contains a Riesz basis of subspaces.

Finally, in Section 10.6 we discover a simple way how to relate the similarity transforms between Laplacians on graphs with elementary similarity transforms between matrices defining the boundary conditions. This main result enables us not only to effectively analyse the problem of quasi-self-adjointness for such graphs but it turns out to be technically useful for self-adjoint Laplacians, too.

10.2 The Laplacian on finite metric graphs

Metric graphs are locally linear one dimensional spaces with singularities at the vertices, and one can think roughly of a metric graph as a union of finitely many finite intervals $[0, a_i]$, with $a_i \in (0, \infty)$, or semi-infinite intervals $[0, \infty)$ glued together at their end points. This intuitive picture is formalised here by recalling from [24, 25, 27] some notation and basic definitions.

10.2.1 Graph as a topological space

A *graph* is a 4-tuple $\mathcal{G} = (\mathcal{V}, \mathcal{I}, \mathcal{E}, \partial)$, where $\mathcal{V}$ denotes the set of *vertices*, $\mathcal{I}$ the set of *internal edges* and $\mathcal{E}$ the set of *external edges*, where the set $\mathcal{E} \cup \mathcal{I}$ is summed up in the notion *edges*. The *boundary map* ∂ assigns to each internal edge $i \in \mathcal{I}$ an ordered pair of vertices $\partial(i) = (\partial_-(i), \partial_+(i)) \in \mathcal{V} \times \mathcal{V}$, where $\partial_-(i)$ is called its *initial vertex* and $\partial_+(i)$ its *terminal vertex*. Each external edge $e \in \mathcal{E}$ is mapped by ∂ onto a single, its initial, vertex. The *degree* $\deg(v)$ of a vertex $v \in \mathcal{V}$ is the number of edges with initial vertex v plus the number of edges with terminal vertex v. A graph is called *finite* if $|\mathcal{V}| + |\mathcal{I}| + |\mathcal{E}| < \infty$ and a finite graph is called *compact* if $\mathcal{E} = \emptyset$.

10.2.2 Graph as a metric space

A graph $\mathcal{G}$ is endowed with the following metric structure. Each internal edge $i \in \mathcal{I}$ is associated with an interval $[0, a_i]$, with $a_i > 0$, such that its initial vertex corresponds to 0 and its terminal vertex to a_i. Each external edge $e \in \mathcal{E}$ is associated to the half line $[0, \infty)$ such that $\partial(e)$ corresponds to 0. The numbers a_i are called *lengths* of the internal edges $i \in \mathcal{I}$ and they are summed up into the vector $\underline{a} = \{a_i\}_{i \in \mathcal{I}} \in (0, \infty)^{|\mathcal{I}|}$. The 2-tuple consisting of a finite graph endowed with a metric structure is called a *metric graph* $(\mathcal{G}, \underline{a})$. The metric on $(\mathcal{G}, \underline{a})$ is defined via minimal path lengths.

10.2.3 Graph as a measure space

Equipping each edge of the metric graph with the one-dimensional Lebesgue measure, we obtain a measure space. Any function $\psi \colon (\mathcal{G}, \underline{a}) \to \mathbb{C}$ can be written as

$$\psi(x_j) = \psi_j(x), \quad \text{where} \quad \psi_j \colon I_j \to \mathbb{C},$$

with

$$I_j = \begin{cases} [0, a_j], & \text{if } j \in \mathcal{I}, \\ [0, \infty), & \text{if } j \in \mathcal{E}. \end{cases}$$

Occasionally we write also $\psi_j(x) = \psi_j(x_j)$. One defines

$$\int_{\mathcal{G}} \psi := \sum_{i \in \mathcal{I}} \int_0^{a_i} \psi(x_i)\, dx_i + \sum_{e \in \mathcal{E}} \int_0^{\infty} \psi(x_e)\, dx_e,$$

where dx_i and dx_e refers to integration with respect to the Lebesgue measure on the intervals $[0, a_i]$ and $[0, \infty)$, respectively.

10.2.4 Graph as a Hilbert space

Given a finite metric graph $(\mathcal{G}, \underline{a})$ one considers the Hilbert space

$$\mathcal{H} \equiv \mathcal{H}(\mathcal{E}, \mathcal{I}, \underline{a}) = \mathcal{H}_{\mathcal{E}} \oplus \mathcal{H}_{\mathcal{I}}, \quad \mathcal{H}_{\mathcal{E}} = \bigoplus_{e \in \mathcal{E}} \mathcal{H}_e, \quad \mathcal{H}_{\mathcal{I}} = \bigoplus_{i \in \mathcal{I}} \mathcal{H}_i,$$

where $\mathcal{H}_j = L^2(I_j; \mathbb{C})$. Hence, the scalar product in $\mathcal{H}$ is given by

$$\langle \psi, \varphi \rangle = \int_{\mathcal{G}} \psi\, \overline{\varphi}.$$

10.2.5 Graph as an energy space

Denote by $\mathcal{W}_j$, $j \in \mathcal{E} \cup \mathcal{I}$ the set of all functions $\psi_j \in \mathcal{H}_j$ which are absolutely continuous with square integrable derivative ψ_j', and set

$$\mathcal{W} = \bigoplus_{j \in \mathcal{E} \cup \mathcal{I}} \mathcal{W}_j. \tag{10.2}$$

With the scalar product defined by

$$\langle \psi, \varphi \rangle_{\mathcal{W}} := \langle \psi', \varphi' \rangle + \langle \psi, \varphi \rangle$$

the space $\mathcal{W}$ becomes a Hilbert space.

By $\mathcal{D}_j$ with $j \in \mathcal{E} \cup \mathcal{I}$ denote the set of all $\psi_j \in \mathcal{H}_j$ such that ψ_j and its derivative ψ_j' are absolutely continuous and its second derivative ψ_j'' is square integrable. Let $\mathcal{D}_j^0$ denote the set of all elements $\psi_j \in \mathcal{D}_j$ with

$$\begin{aligned} &\psi_j(0) = 0, \quad \psi'(0) = 0, \quad \text{for } j \in \mathcal{E}, \\ &\psi_j(0) = 0, \quad \psi'(0) = 0, \quad \psi_j(a_j) = 0, \ \psi'(a_j) = 0, \ \text{for } j \in \mathcal{I}. \end{aligned}$$

The sets

$$\mathcal{D} = \bigoplus_{j \in \mathcal{E} \cup \mathcal{I}} \mathcal{D}_j \quad \text{and} \quad \mathcal{D}^0 = \bigoplus_{j \in \mathcal{E} \cup \mathcal{I}} \mathcal{D}_j^0$$

together with the scalar product defined by

$$\langle \psi, \varphi \rangle_{\mathcal{D}} := \langle \psi'', \varphi'' \rangle + \langle \psi, \varphi \rangle_{\mathcal{W}}$$

become Hilbert spaces, such that $\mathcal{D}^0 \subset \mathcal{D}$ is closed.

10.2.6 Graph as a Laplacian

Let Δ be the differential operator

$$(\Delta \psi)_j (x) = \frac{d^2}{dx^2} \psi_j(x), \quad j \in \mathcal{E} \cup \mathcal{I}, \quad x \in I_j,$$

with domain $\mathcal{D}$, and Δ^0 its restriction on the domain $\mathcal{D}^0$. It is known that the operator Δ^0 is a closed symmetric operator with deficiency indices (d, d), where

$$d := |\mathcal{E}| + 2|\mathcal{I}|, \tag{10.3}$$

and its Hilbert space adjoint is $(\Delta^0)^* = \Delta$; see, *e.g.*, [9, Sec. 4.8].

Any closed extension $-\widetilde{\Delta}$ of $-\Delta^0$ satisfying

$$\Delta^0 \subset \widetilde{\Delta} \subset \Delta \tag{10.4}$$

will be called the *Laplacian* on $(\mathcal{G}, \underline{a})$. Self-adjoint Laplacians on graphs are well studied. The aim of this paper is to discuss extensions of $-\Delta^0$ which are not necessarily self-adjoint.

The extensions $\widetilde{\Delta}$ of Δ^0 with (10.4) can be discussed in terms of boundary or matching conditions imposed at the endpoints of the edges. For this purpose one defines for $\psi \in \mathcal{D}$ the vectors of boundary values

$$\underline{\psi} = \begin{bmatrix} \{\psi_e(0)\}_{e \in \mathcal{E}} \\ \{\psi_i(0)\}_{i \in \mathcal{I}} \\ \{\psi_i(a_i)\}_{i \in \mathcal{I}} \end{bmatrix} \quad \text{and} \quad \underline{\psi}' = \begin{bmatrix} \{\psi_e'(0)\}_{e \in \mathcal{E}} \\ \{\psi_i'(0)\}_{i \in \mathcal{I}} \\ \{-\psi_i'(a_i)\}_{i \in \mathcal{I}} \end{bmatrix}.$$

One introduces the auxiliary Hilbert space

$$\mathcal{K} \equiv \mathcal{K}(\mathcal{E}, \mathcal{I}) = \mathcal{K}_{\mathcal{E}} \oplus \mathcal{K}_{\mathcal{I}}^- \oplus \mathcal{K}_{\mathcal{I}}^+$$

with $\mathcal{K}_{\mathcal{E}} = \mathbb{C}^{|\mathcal{E}|}$ and $\mathcal{K}_{\mathcal{I}}^{(\pm)} = \mathbb{C}^{|\mathcal{I}|}$. One sets

$$[\psi] := \underline{\psi} \oplus \underline{\psi}' \in \mathcal{K} \oplus \mathcal{K}.$$

Any extension $\widetilde{\Delta}$ with (10.4) can be associated with a subspace $\mathcal{M} \subset \mathcal{K}^2 := \mathcal{K} \oplus \mathcal{K}$ such that $\widetilde{\Delta} = \Delta(\mathcal{M})$ is the restriction of Δ to the domain

$$\mathsf{D}(\Delta(\mathcal{M})) = \{\psi \in \mathcal{D} \mid [\psi] \in \mathcal{M}\}.$$

10.3 Classification of boundary conditions

There are various ways to parametrise the subspaces $\mathcal{M} \subset \mathcal{K}^2$. In the following some parametrisations are discussed starting with self-adjoint boundary conditions and then transferring the methods to non-self-adjoint ones.

Given linear maps A, B in $\mathcal{K}$, one defines

$$(A,\, B)\colon \mathcal{K}^2 \to \mathcal{K}, \quad (A,\, B)(\chi_1 \oplus \chi_2) = A\chi_1 + B\chi_2 \quad \text{for } \chi_1, \chi_2 \in \mathcal{K},$$

and sets

$$\mathcal{M}(A, B) := \mathsf{N}(A,\, B).$$

If $\dim \mathcal{M} \geq d$ there are appropriate operators A, B acting in $\mathcal{K}$ such that $\mathcal{M} = \mathcal{M}(A, B)$, and then an equivalent description of $\mathsf{D}(\Delta(\mathcal{M}))$ is that it contains all functions $\psi \in \mathcal{D}$ satisfying the linear *boundary conditions*

$$A\underline{\psi} + B\underline{\psi}' = 0. \tag{10.5}$$

In this case one also writes equivalently $\Delta(\mathcal{M}) = \Delta(A, B)$. Note that the parametrisation by the matrices A and B is not unique. Indeed, operators $\Delta(A, B)$ and $\Delta(A', B')$ agree if and only if the corresponding spaces $\mathcal{M}(A, B)$ and $\mathcal{M}(A', B')$ agree. Therefore we introduce

Definition 10.1. Boundary conditions defined by A, B and A', B' are called *equivalent* if $\mathcal{M}(A, B) = \mathcal{M}(A', B')$.

Notice that the boundary conditions are equivalent if and only if there exists an invertible operator C in $\mathcal{K}$ such that simultaneously

$$A' = CA \quad \text{and} \quad B' = CB.$$

10.3.1 Self-adjoint boundary conditions

Recall that any self-adjoint realisation of Δ can be parametrised as $\Delta(A, B)$, where the matrices A and B satisfy $AB^* = BA^*$ and $\dim \mathcal{M}(A, B) = d$, where d is defined in (10.3); see, *e.g.*, [23, Lem. 2.2 and below it].

It is a classical result that there is a one-to-one correspondence between unitary operators U in $\mathcal{K}$ and self-adjoint realisations of Δ. More precisely, any self-adjoint extension of Δ^0 can be defined by the boundary conditions

$$-\frac{1}{2}\,(U - \mathbb{1})\,\underline{\psi} + \frac{1}{2ik}\,(U + \mathbb{1})\,\underline{\psi}' = 0, \tag{10.6}$$

for $k > 0$; see, *e.g.*, [17, Sec. 3].

The link between the parametrisation by unitary operators U and the one by matrices A and B in (10.5) is given by a Cayley transform. For A, B defining a self-adjoint Laplacian, consider, for $k \in \mathbb{C} \setminus \{0\}$ such that $A + ikB$ is invertible, the transform

$$\mathfrak{S}(k, A, B) := -\,(A + ikB)^{-1}\,(A - ikB)\,. \tag{10.7}$$

For $k > 0$ the operator $\mathfrak{S}(k, A, B)$ is unitary [23, Thm. 2.1] and one can choose $U = \mathfrak{S}(k, A, B)$ in (10.6), *cf* [24, p. 209]. For self-adjoint Laplacians on graphs with $\mathcal{I} = \emptyset$ the matrix $\mathfrak{S}(A, B, k)$ admits also the interpretation as the *scattering matrix* for a certain scattering pair [25].

10.3.2 Regular boundary conditions

The transform $\mathfrak{S}(k, A, B)$ can be defined for non-self-adjoint boundary conditions as well whenever $A + ikB$ is invertible, and then $\mathfrak{S}(k, A, B)$ is independent of the concrete choice of A, B representing $\mathcal{M} = \mathcal{M}(A, B)$. So, whenever $A + ikB$ is invertible for $k \in \mathbb{C} \setminus \{0\}$ one re-obtains from $\mathfrak{S}(k, A, B)$ equivalent boundary conditions of the form (10.5) by

$$A_{\mathfrak{S}} := -\frac{1}{2}\,(\mathfrak{S}(k, A, B) - \mathbb{1}) \quad \text{and} \quad B_{\mathfrak{S}} := \frac{1}{2ik}\,(\mathfrak{S}(k, A, B) + \mathbb{1})\,. \tag{10.8}$$

This follows from the equalities

$$(A + ikB)A_{\mathfrak{S}} = A \quad \text{and} \quad (A + ikB)B_{\mathfrak{S}} = B$$

used in [27, proof of Lem. 3.4]. A necessary condition for the definition of $\mathfrak{S}(k, A, B)$ is that $\dim \mathcal{M}(A, B) = d$, but this is not sufficient. Actually, since $\det(A + ikB)$ is a polynomial in k of degree at the most d, $A + ikB$ is not invertible either for every $k \in \mathbb{C}$ or only for finitely many values $k \in \mathbb{C}$.

Definition 10.2. Boundary conditions (10.5) defined by A, B with $\dim \mathcal{M}(A, B) = d$ such that $A + ikB$ is invertible for some $k \in \mathbb{C}$ are called *regular* boundary conditions.

10.3.3 Other notions of regular boundary conditions

The reader is warned that there exist further parametrisations and classifications of boundary conditions for the second derivative operator acting on intervals. For instance, the classification given in [13, Sec. XIX.4] is based on the structure of certain determinants related to the secular equation, and this gives rise to an alternative regularity assumption [13, Hypothesis XIX.4.1] on boundary conditions. The aim in [13] is to define *spectral operators* and the regularity hypothesis goes back to [7, 8].

That the regularity hypothesis formulated in [13, Hypothesis XIX.4.1] does not agree with the notion of regular boundary conditions introduced in our Definition 10.2 follows already from [13, Ex. XIX.6(d)], which is discussed here as Example 10.6 below. The boundary conditions given in [13, Ex. XIX.6(d)] are called *intermediate* boundary conditions and are an example of a class of boundary conditions not satisfying the regularity hypothesis [13, Hypothesis XIX.4.1], see also [8, p.383], whereas they are regular in the sense introduced here.

In general it seems difficult to make precise statement on the secular equation for – in our sense – regular boundary conditions. More generally, when considering non-compact graphs, *i.e.* $\mathcal{E} \neq \emptyset$, there is no straightforward generalisation of the regularity hypothesis of [13, Sec. XIX.4] since it is dealing with operators with discrete spectrum.

10.3.4 Irregular boundary conditions

Boundary conditions defined by A, B with $\dim \mathcal{M}(A,B) = d$ which are not regular will be called *irregular*. We do not include the situations $\dim \mathcal{M}(A,B) \neq d$ into our notion of irregular boundary conditions, since they are not spectrally interesting. Indeed, it follows from Proposition 10.5 below that $\sigma(-\Delta(A,B)) = \mathbb{C}$ whenever $\dim \mathcal{M}(A,B) \neq d$.

The class of regular boundary conditions covers many relevant and interesting cases, whereas the irregular boundary conditions seem to be rather pathological. Indeed, the latter are typically associated with operators that have empty resolvent set or empty spectrum, even if $\dim \mathcal{M}(A,B) = d$ holds.

Example 10.1 (Indefinite Laplacian, no resolvent set)**.** Consider the boundary conditions (10.5) given by

$$A = \begin{pmatrix} 1 & -1 \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad B = \begin{pmatrix} 0 & 0 \\ 1 & -1 \end{pmatrix}$$

for the graph $\mathcal{G} = (V, \partial, \mathcal{E})$ consisting of two external edges $\mathcal{E} = \{e_1, e_2\}$ and one vertex $\partial(e_1) = \partial(e_2)$. Identifying this graph with the real line, the operator $-\Delta(A,B)$ corresponds to the indefinite operator

$$-\operatorname{sign}(x)\frac{d}{dx}\operatorname{sign}(x)\frac{d}{dx} \qquad \text{on} \qquad L^2(\mathbb{R})$$

with its natural domain $\{\psi \in W^{1,2}(\mathbb{R}) \,|\, (\psi' \operatorname{sign})' \in L^2(\mathbb{R})\}$. This operator is studied within the framework of Krein space theory in [36, Sec. 5].

This example demonstrates in particular that $\dim \mathcal{M}(A,B) = d$ is a necessary but not a sufficient condition for A, B to define regular boundary conditions. Indeed, $\dim \mathcal{M}(A,B) = 2 = d$ in this example, while $A + ikB$ is invertible for no complex k. (As a consequence, the statement in [27, observation below Ass. 2.1] is not correct in general, but it holds for the boundary conditions defining m-accretive operators studied there.)

Note that the equation $\det(A + ikB) = 0$ with $\Im k > 0$ is the secular equation for the spectral problem associated with $-\Delta(A,B)$, *cf* Subsection 10.4.1 below. Therefore the spectrum of the operator described in the present example is entire $\mathbb{C}$. This fact will be explained also in Subsection 10.6.4 by means of a similarity transform.

Example 10.2 (Totally degenerate boundary conditions, no spectrum)**.** This example is overtaken from [13, Sec. XIX.6(b)]. Consider the interval $[0,1]$ and the irregular boundary conditions defined by

$$A = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \quad \text{and} \quad B = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}.$$

Then $\dim \mathcal{M}(A,B) = 2 = d$ and the boundary conditions correspond to

$$\psi(0) = 0 \quad \text{and} \quad \psi'(0) = 0,$$

whereas on the other endpoint no boundary conditions are imposed. By integration one can show that this operator is boundedly invertible, and for the compact embedding $\mathcal{D} \hookrightarrow \mathcal{H}$ the inverse is compact, and hence the operator $-\Delta(A,B)$ has only point spectrum. However, a direct computation shows that for these boundary conditions there are no eigenvalues, and therefore the spectrum of $-\Delta(A,B)$ is empty.

By inspection of the previous examples, it is straightforward to identify the mechanism which is behind the irregularity of the boundary conditions.

Proposition 10.1. *Let A, B be maps in $\mathcal{K}$ such that* $\dim \mathcal{M}(A,B) = d$. *Then A, B define irregular boundary conditions if and only if*

$$\mathsf{N}A \cap \mathsf{N}B \neq \{0\}.$$

Proof. If $\mathsf{N}A \cap \mathsf{N}B \neq \{0\}$, then for a non-zero $\underline{\psi} \in \mathsf{N}A \cap \mathsf{N}B$ one has $(A + ikB)\underline{\psi} = 0$ for any $k \in \mathbb{C}$. The other way round, if $A + ikB$ is not invertible for any $k \in \mathbb{C}$, then $\mathsf{N}A \neq \{0\}$, since otherwise one could consider $\mathbb{1} + ikA^{-1}B$ which is invertible for k sufficiently small. So, for non-zero $\underline{\psi} \in \mathsf{N}A$ one has $ikB\underline{\psi} = 0$ for any $k \in \mathbb{C}$ and hence $\underline{\psi} \in \mathsf{N}B$, which proves that $\mathsf{N}A \cap \mathsf{N}B \neq \{0\}$. □

A possible generalisation of Example 10.1 to more complex graphs is given by the following example.

Example 10.3 (A generalisation of Example 10.1)**.** Consider a star graph with $\mathcal{I} = \emptyset$ and subdivision of the external edges $\mathcal{E} = \mathcal{E}_+ \dot{\cup} \mathcal{E}_-$ together with the boundary conditions defined by

$$A = \begin{bmatrix} 1 & -1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & -1 & \cdots & 0 & 0 \\ 0 & 0 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & -1 \\ 0 & 0 & 0 & \cdots & 0 & 0 \end{bmatrix}, \qquad B = \begin{bmatrix} 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & 0 \\ 1 & \cdots & 1 & \cdots & -1 & -1 \end{bmatrix},$$

where in the last row of B for each edge in $\mathcal{E}_+$ stands a $+1$ and for each edge in $\mathcal{E}_-$ a -1. To paraphrase, these boundary conditions guarantee that functions are continuous at the central vertex and that the sum of the outward directed derivatives evaluated at the positive incident edges equals the sum of the outward directed derivatives evaluated at the negative incident edges. These boundary conditions define an operator which is self-adjoint in a certain Krein space [19, Sec. 4]. The kernel of A is spanned by the vector w with $(w)_i = 1$, for all $i \in \{1, \ldots, |\mathcal{E}|\}$. Hence, by Proposition 10.1, for $|\mathcal{E}_+| = |\mathcal{E}_-|$ the boundary conditions defined by A, B are irregular and for $|\mathcal{E}_+| \neq |\mathcal{E}_-|$ they are regular. For example, in the case $|\mathcal{E}_+| = 2$ and $|\mathcal{E}_-| = 1$ one obtains the k-independent "scattering matrix"

$$\mathfrak{S}(k, A, B) = \begin{bmatrix} 1 & 2 & -2 \\ 2 & 1 & -2 \\ 2 & 2 & -3 \end{bmatrix}.$$

Remark 10.1. Let the boundary conditions be *local*, *i.e.*

$$\mathcal{M} = \bigoplus_{v \in \mathcal{V}} \mathcal{M}_v,$$

where $\mathcal{M}_v$ are subspaces of $\mathcal{K}_v^2$, the space of boundary values associated with the endpoints of the edges incident in the vertex v, *cf* [27, Def. 2.6]. Then it is a direct consequence of Proposition 10.1 that the boundary conditions are regular if and only if the boundary conditions at each vertex are regular, and irregular if at least at one vertex the boundary conditions are irregular.

10.3.5 m-sectorial boundary conditions

In [34, Corol. 5] a further way how to parametrise self-adjoint Laplacians on graphs is proposed. It is given in terms of an orthogonal projection P acting in $\mathcal{K}$ and a self-adjoint operator L acting in the subspace $\mathsf{N}P$. For any self-adjoint Laplacian one has $-\Delta(A, B) = -\Delta(A', B')$ with $A' = L + P$ and $B' = P^\perp$, where using $\mathsf{R}B^* = (\mathsf{N}B)^\perp$ one sets

$$L = (B\,|_{\mathsf{R}B^*})^{-1}\, AP^\perp$$

and P denotes the orthogonal projector onto $\mathsf{N}B \subset \mathcal{K}$ and $P^\perp = \mathbb{1} - P$ is the complementary projector. This parametrisation is unique in contrast to that using matrices A, B, and additionally it is convenient when considering forms associated with operators, *cf* [34, Thms. 6 and 9].

Inspired by the self-adjoint situation, for a given projector P and a not necessarily self-adjoint operator L acting in $\mathsf{N}P$, *i.e.* $L = P^\perp L P^\perp$, let us consider $-\Delta(\mathcal{M})$ with $\mathcal{M} = \mathcal{M}(L+P, P^\perp)$. According to [18, Thm. 3.1], this operator is m-sectorial and associated with the closed sectorial form $\delta_{P,L}$ defined by

$$\begin{aligned} \delta_{P,L}[\psi] &= \int_{\mathcal{G}} |\psi'|^2 - \langle L P^\perp \underline{\psi}, P^\perp \underline{\psi} \rangle_{\mathcal{K}}, \\ \psi &\in \mathsf{D}(\delta_{P,L}) = \{\varphi \in \mathcal{W} \mid P\underline{\varphi} = 0\}, \end{aligned} \tag{10.9}$$

where $\mathcal{W}$ denotes the Sobolev space (10.2).

The question when $\mathcal{M}(A,B)$ with $\dim \mathcal{M}(A,B) = d$ admits an equivalent parametrisation in terms of a projector P and an operator L acting in $\mathsf{N}P$ such that $\mathcal{M}(A,B) = \mathcal{M}(L+P, P^\perp)$ is discussed in [18]. It turns out that this is possible if and only if $-\Delta(A,B)$ is m-sectorial. Furthermore, if $\mathcal{M}(A,B)$ does not admit such a parametrisation, then the numerical range of $-\Delta(A,B)$ is entire $\mathbb{C}$, see [18, Lem. 4.3]. Therefore, here we call boundary conditions defined by P and L as described above *m-sectorial*. Descriptive examples of such boundary conditions are δ-interactions with generally complex coupling parameters. Note that in order to apply any kind of form methods one needs at least m-sectorial boundary conditions.

Example 10.4 (Complex δ-interaction)**.** Consider a graph with $\mathcal{I} = \emptyset$ and $|\mathcal{E}| \geq 2$. Assume that the boundary conditions are defined up to equivalence by

$$A = \begin{bmatrix} 1 & -1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & -1 & \cdots & 0 & 0 \\ 0 & 0 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & -1 \\ -\gamma & 0 & 0 & \cdots & 0 & 0 \end{bmatrix}, \qquad B = \begin{bmatrix} 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & 0 \\ 1 & 1 & 1 & \cdots & 1 & 1 \end{bmatrix},$$

where $\gamma \in \mathbb{C}$. For real γ one can represent the boundary conditions equivalently by the m-sectorial boundary conditions defined by $P = \mathbb{1} - P^\perp$, where $P^\perp$ is the rank one projector onto $(\mathsf{N}B)^\perp$, and $L = -\frac{\gamma}{|\mathcal{E}|} P^\perp$, *cf* [34, Sec. 3.2.1]. A direct calculation shows that this carries over to the case of complex coupling parameters γ. The operator $-\Delta(A,B)$ is associated with the quadratic form defined by

$$\delta_{P,L}[\psi] = \int_{\mathcal{G}} |\psi'|^2 + \frac{\gamma}{|\mathcal{E}|} |\underline{\psi}|^2, \quad \psi \in \mathsf{D}(\delta_{P,L}) = \{\psi \in \mathcal{W} \mid P\underline{\psi} = 0\}.$$

It is proved in [18] that the boundary conditions of the form (10.5) defined by matrices A, B can be substituted by an equivalent parametrisation using m-sectorial boundary conditions if and only if

$$\dim \mathcal{M}(A,B) = d \quad \text{and} \quad QAP^\perp = 0, \tag{10.10}$$

where Q is the orthogonal projector onto $(\mathsf{R}B)^\perp$ and $P^\perp$ the orthogonal projector onto $(\mathsf{N}B)^\perp$. This is due to the fact that the evaluation at the vertices of the derivatives cancel out in the corresponding quadratic form if and only if $QAP^\perp = 0$.

Note that $L + P + ikP^\perp$ has a block diagonal form with respect to the decomposition of $\mathcal{K}$ into $\mathsf{R}P$ and $\mathsf{R}P^\perp$. Thus $L + P + ikP^\perp$ is invertible for $|k| > \|L\|$. Consequently, the parametrisation by the transform $\mathfrak{S}(k, L+P, P^\perp)$ is admissible, whereas the converse is not true: from $A + ikB$ invertible, in general, it does not follow that there are equivalent m-sectorial boundary conditions. This is illustrated by the following examples.

Example 10.5 (From Kirchhoff to wild aperiodic boundary conditions)**.** Let $\mathcal{G} = (\mathcal{V}, \partial, \mathcal{E})$ be a graph consisting of two external edges $\mathcal{E} = \{e_1, e_2\}$ and one vertex $\partial(e_1) = \partial(e_2)$. Consider the boundary conditions defined by

$$A_\tau = \begin{pmatrix} 1 & -e^{i\tau} \\ 0 & 0 \end{pmatrix} \quad \text{and} \quad B_\tau = \begin{pmatrix} 0 & 0 \\ 1 & e^{-i\tau} \end{pmatrix},$$

for $\tau \in [0, \pi/2]$. Identifying the graph with the real line and the vertex with zero, the boundary conditions correspond to

$$\psi(0+) = e^{i\tau}\psi(0-) \quad \text{and} \quad \psi'(0+) = e^{-i\tau}\psi'(0-).$$

This example is included in the study of $\mathcal{PT}$-symmetric point interactions in [2] and was further investigated in [3] and [44, Chap. 2.5].

The matrix $A_\tau + ikB_\tau$ is invertible for $\tau \in [0, \pi/2)$ and $k \neq 0$, hence A_τ, B_τ define regular boundary conditions for $\tau \in [0, \pi/2)$. For the Cayley transform

$$\mathfrak{S}(A_\tau, B_\tau, k) = -(A_\tau + ikB_\tau)^{-1}(A_\tau - ikB_\tau), \quad \tau \in [0, \pi/2),$$

an explicit computation yields the k-independent matrix

$$\mathfrak{S}(A_\tau, B_\tau, k) = \frac{1}{\cos(\tau)} \begin{bmatrix} i\sin(\tau) & 1 \\ 1 & -i\sin(\tau) \end{bmatrix}.$$

The operator $\mathfrak{S}(A_\tau, B_\tau, k)$ is unitary (with eigenvalues $+1$ and -1) only for $\tau = 0$, where it defines the so-called standard or Kirchhoff boundary conditions.

On the other hand, for $\tau = \pi/2$ one has $\det(A_{\pi/2} + ikB_{\pi/2}) = 0$ for any $k \in \mathbb{C}$, and therefore $A_{\pi/2}, B_{\pi/2}$ define irregular boundary conditions. Furthermore one has $\sigma_{\mathrm{p}}(-\Delta(A_{\pi/2}, B_{\pi/2})) = \mathbb{C}\backslash[0,\infty)$, because of (10.15) below. This reproduces the results obtained in [3, Thm. 2] and [44, Chap. 2.5].

Explicit computation yields

$$\mathsf{R}B_\tau = \operatorname{span}\left\{\begin{pmatrix} 0 \\ 1 \end{pmatrix}\right\}, \qquad (\mathsf{R}B_\tau)^\perp = \operatorname{span}\left\{\begin{pmatrix} 1 \\ 0 \end{pmatrix}\right\},$$
$$\mathsf{N}B_\tau = \operatorname{span}\left\{\begin{pmatrix} 1 \\ -e^{i\tau} \end{pmatrix}\right\}, \qquad (\mathsf{N}B_\tau)^\perp = \operatorname{span}\left\{\begin{pmatrix} 1 \\ e^{i\tau} \end{pmatrix}\right\},$$

and therefore, with Q_τ being the orthogonal projector onto $(\mathsf{R}B_\tau)^\perp$ and $P_\tau^\perp$ being the orthogonal projector onto $(\mathsf{N}B_\tau)^\perp$, one has

$$Q_\tau A_\tau P_\tau^\perp = \frac{1}{2}\begin{pmatrix} 1 - e^{2i\tau} & e^{-i\tau} - e^{i\tau} \\ 0 & 0 \end{pmatrix} \neq 0, \quad \text{for } \tau \in (0, \pi/2].$$

The criterion in (10.10) implies that for $\tau \in (0, \pi/2]$ there is no equivalent representation of A_τ, B_τ by m-sectorial boundary conditions. This can be illustrated also by considering the quadratic form defined by the operator $-\Delta(A_\tau, B_\tau)$ which by integrating by parts and inserting the boundary conditions simplifies to become

$$\langle -\Delta(A_\tau, B_\tau)\psi, \psi\rangle = \int_{\mathcal{G}} |\psi'|^2 + (1 - e^{2i\tau})\psi_2(0)\overline{\psi_2'(0)}$$

for every $\psi \in \mathsf{D}(-\Delta(A_\tau, B_\tau))$. In particular, the derivative term cannot be avoided, and the numerical range is entire $\mathbb{C}$ for all $\tau \in (0, \pi/2]$.

Despite of the wild numerical range properties, in Section 10.6.4 we shall show that for $\tau \in [0, \pi/2)$ the operator $-\Delta(A_\tau, B_\tau)$ is similar to the self-adjoint Laplacian $-\Delta(A_0, B_0)$, and hence its spectrum is $[0, \infty)$. Such a similarity relation is of course impossible for $\tau = \pi/2$ because the spectrum is entire $\mathbb{C}$.

The analogous operator on the graph with two internal edges of the same length defined by boundary conditions A_τ, B_τ at the central vertex and Dirichlet boundary conditions at the endpoints exhibit similar pathological behaviours, see [44, Chap. 2.5].

Example 10.6 (Intermediate boundary conditions)**.** Consider the interval $[0, 1]$ and the regular boundary conditions defined by

$$A = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad \text{and} \quad B = \begin{bmatrix} 0 & 0 \\ -1 & 0 \end{bmatrix},$$

i.e. $\psi(0) = 0$ and $\psi(1) - \psi'(0) = 0$. Then $\dim \mathcal{M}(A, B) = 2$ and

$$QAP^\perp = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \neq 0.$$

Hence the boundary conditions are not m-sectorial. One has

$$\langle -\Delta(A, B)\psi, \psi\rangle = \int_0^1 |\psi'|^2 - \psi'(0)\overline{\psi'(1)}$$

for every $\psi \in \mathsf{D}(-\Delta(A, B))$. This example can be found in [8, p.383] as well as in [13, Ex. XIX.6(d)], where the boundary conditions are called *intermediate*.

Using the methods developed in the forthcoming Section 10.4 one can show that the spectrum of $-\Delta(A, B)$ consists only of eigenvalues of geometric multiplicity one, where each eigenvalue is a solution of $\sin(k) = k$, $k \in \mathbb{C}$.

10.3.6 Adjoint boundary conditions

Consider for $\mathcal{M} \subset \mathcal{K}^2$ the possibly non-self-adjoint operator $\Delta(\mathcal{M})$. Since $\Delta^0 \subset \Delta(\mathcal{M}) \subset \Delta$ it follows for the adjoint operator that $\Delta(\mathcal{M})^* = \Delta(\mathcal{M}^*)$ for an appropriate subspace $\mathcal{M}^* \subset \mathcal{K}^2$, and hence also the adjoint operator can be described by means of boundary conditions.

Proposition 10.2. *Let $\mathcal{M} \subset \mathcal{K}^2$, then $\Delta(\mathcal{M})^* = \Delta(\mathcal{M}^*)$ with*

$$\mathcal{M}^* = (J\mathcal{M})^{\perp}, \quad \text{where } J = \begin{bmatrix} 0 & \mathbb{1}_{\mathcal{K}} \\ -\mathbb{1}_{\mathcal{K}} & 0 \end{bmatrix}$$

defines a map in $\mathcal{K}^2$.

Proof. By definition, the adjoint of $\Delta(\mathcal{M})$ in the Hilbert space $\mathcal{H}$ is the operator defined on

$$\mathsf{D}(\Delta(\mathcal{M})^*) = \{\psi \in \mathcal{H} \mid \exists \varphi \in \mathcal{H}, \forall \eta \in \mathsf{D}(\Delta(\mathcal{M})), \ \langle \psi, \Delta(\mathcal{M})\eta \rangle = \langle \varphi, \eta \rangle\},$$

by $\Delta(\mathcal{M})^*\psi = \varphi$. It follows from (10.4) that $\Delta^0 \subset \Delta(\mathcal{M})^* \subset \Delta$, and hence $\Delta(\mathcal{M})^*$ is also a realisation of Δ defined by means of boundary conditions. Consequently, $\Delta(\mathcal{M})^*\psi = \Delta\psi$ and $\mathcal{D}^0 \subset \mathsf{D}(\Delta(\mathcal{M})^*) \subset \mathcal{D}$. It remains to determine the domain of $\Delta(\mathcal{M})^*$ by specifying the boundary conditions. An integration by parts yields

$$\langle \psi, \Delta(\mathcal{M})\eta \rangle - \langle \Delta\psi, \eta \rangle = \langle J[\psi], [\eta] \rangle_{\mathcal{K}^2} \tag{10.11}$$

for every $\eta \in \mathsf{D}(\Delta(\mathcal{M}))$ and $\psi \in \mathcal{D}$. Define

$$[\cdot]_{\mathcal{M}} \colon \mathsf{D}(\Delta(\mathcal{M})) \to \mathcal{K}^2, \quad [\eta]_{\mathcal{M}} = [\eta],$$

and observe that the range of $[\cdot]_{\mathcal{M}}$ is $\mathcal{M}$, and that the boundary term (10.11) vanishes identically for all $\psi \in \mathsf{D}(\Delta(\mathcal{M}^*))$. Hence $\Delta(\mathcal{M}^*) \subset \Delta(\mathcal{M})^*$. Noticing that the boundary term in (10.11) vanishes for all $\eta \in \mathsf{D}(\Delta(\mathcal{M}))$ if and only if $J[\psi] \perp \mathcal{M}$ and using that J is unitary, we have $[\psi] \perp J\mathcal{M}$ for $\psi \in \mathsf{D}(\Delta(\mathcal{M})^*)$. Consequently, $\Delta(\mathcal{M})^* \subset \Delta(\mathcal{M}^*)$, which proves the claim. □

Corollary 10.1. *Let $\mathcal{M} \in \mathcal{K}^2$, then* $\dim \mathcal{M} + \dim \mathcal{M}^* = 2d$.

Proof. As J is unitary one has $\dim \mathcal{M} = \dim J\mathcal{M}$, from which the claim follows. □

10.3.7 Adjoints for regular boundary conditions

Searching for boundary conditions that define Laplacians with non-empty resolvent set, one needs by the forthcoming Proposition 10.5 the condition $\dim \mathcal{M} = d$, and therefore this case is of particular interest. For regular boundary conditions the parametrisation in terms of $\mathfrak{S}(k, A, B)$ is convenient for this purpose.

Proposition 10.3. *Let A, B be such that $\dim \mathcal{M}(A, B) = d$ and $A + ikB$ is invertible for the number $k \neq 0$. Then an equivalent parametrisation of $\Delta(A, B)$ is given by*

$$A_{\mathfrak{S}} := -\frac{1}{2}\left(\mathfrak{S}(k, A, B) - \mathbb{1}\right) \quad \text{and} \quad B_{\mathfrak{S}} := \frac{1}{2ik}\left(\mathfrak{S}(k, A, B) + \mathbb{1}\right)$$

using $\mathfrak{S}(k, A, B) = -(A + ikB)^{-1}(A - ikB)$, and the adjoint operator $\Delta(\mathcal{M})^* = \Delta(\mathcal{M}^*)$ is defined by $\mathcal{M}^* = \mathcal{M}(A', B')$, where

$$A' := -\frac{1}{2}\left(\mathfrak{S}(k, A, B)^* - \mathbb{1}\right) \quad \text{and} \quad B' := \frac{1}{-2i\overline{k}}\left(\mathfrak{S}(k, A, B)^* + \mathbb{1}\right).$$

Proof. The fact that $A_{\mathfrak{S}}, B_{\mathfrak{S}}$ define equivalent boundary conditions has been discussed already in Subsection 10.3.2.

Let us first prove that $\dim \mathcal{M}(A', B') = d$ for the operators A', B' given in the proposition. Assume that $\dim \mathcal{M}(A', B') > d$. Then

$$\mathcal{M}(A', B')^{\perp} = \mathsf{R}\begin{bmatrix} (A')^* \\ (B')^* \end{bmatrix} \quad \text{and} \quad \dim \mathcal{M}(A', B')^{\perp} < d.$$

Therefore,

$$\mathsf{N}\begin{bmatrix} (A')^* \\ (B')^* \end{bmatrix} = \mathsf{N}(A')^* \cap \mathsf{N}(B')^* \neq \{0\},$$

cf [27, Ass. 2.1 and below]. Note that

$$A' = A_{\mathfrak{S}}^* \quad \text{and} \quad B' = B_{\mathfrak{S}}^*,$$

and hence $\mathsf{N}A_{\mathfrak{S}} \cap \mathsf{N}B_{\mathfrak{S}} \neq \{0\}$, which implies $\det(A_{\mathfrak{S}} + ikB_{\mathfrak{S}}) = 0$ for all $k \in \mathbb{C}$. This is a contradiction to the assumption that A, B define regular boundary conditions. Hence $\dim \mathcal{M}(A', B') = d$.

Now one shows that $\mathcal{M}^* = \mathcal{M}(A', B')$, where $\mathcal{M}^*$ is given in Proposition 10.2. By the equivalence of boundary conditions, one has $\mathcal{M}(A, B) = \mathcal{M}(A_{\mathfrak{S}}, B_{\mathfrak{S}})$. Note that $J\mathcal{M}(A_{\mathfrak{S}}, B_{\mathfrak{S}}) = \mathcal{M}(B_{\mathfrak{S}}, -A_{\mathfrak{S}})$. Hence

$$(J\mathcal{M}(A_{\mathfrak{S}}, B_{\mathfrak{S}}))^{\perp} = \mathsf{R}\begin{bmatrix} B_{\mathfrak{S}}^* \\ -A_{\mathfrak{S}}^* \end{bmatrix} \quad \text{and} \quad \mathcal{M}(A', B')^{\perp} = \mathsf{R}\begin{bmatrix} (A')^* \\ (B')^* \end{bmatrix}.$$

Observe that

$$\begin{aligned} \left\langle \begin{bmatrix} B_{\mathfrak{S}}^* \underline{\psi} \\ -A_{\mathfrak{S}}^* \underline{\psi} \end{bmatrix}, \begin{bmatrix} (A')^* \underline{\varphi} \\ (B')^* \underline{\varphi} \end{bmatrix} \right\rangle_{\mathcal{K}^2} &= -\frac{1}{4ik} \left\langle \underline{\psi}, \left(\mathfrak{S}^2 - \mathbb{1}\right) \underline{\varphi} \right\rangle_{\mathcal{K}} + \frac{1}{4ik} \left\langle \psi, \left(\mathfrak{S}^2 - \mathbb{1}\right) \varphi \right\rangle_{\mathcal{K}} \\ &= 0 \end{aligned}$$

for all $\underline{\psi}, \underline{\varphi} \in \mathcal{K}$, where $\mathfrak{S} = \mathfrak{S}(k, A, B)$. Hence $(J\mathcal{M}(A_{\mathfrak{S}}, B_{\mathfrak{S}}))^{\perp} \perp \mathcal{M}(A', B')^{\perp}$, and since both spaces have dimension equal to d one obtains $(J\mathcal{M}(A_{\mathfrak{S}}, B_{\mathfrak{S}}))^{\perp} = \mathcal{M}(A', B')$. Applying Proposition 10.2 yields the claim. ☐

As a consequence, one obtains for m-sectorial operators the following

Corollary 10.2. *Let P be an orthogonal projector in $\mathcal{K}$, $P^{\perp} = \mathbb{1} - P$ and L and operator with $L = P^{\perp}LP^{\perp}$, then*

$$\Delta(P + L, P^{\perp})^* = \Delta(P + L^*, P^{\perp}).$$

10.3.8 Approximation of boundary conditions

One can ask which boundary conditions are “close to each other”, and for answering this question properly one has to decide in which topology it is raised. Here, boundary conditions with the same dimension are compared to each other. Let us thus consider the set of subspaces $\mathcal{M} \subset \mathcal{K}^2$ with $\dim \mathcal{M} = n$; this is the Grassmann manifold $\mathrm{Gr}(2d, n)$. For a subspace $\mathcal{M} \subset \mathcal{K}^2$ denote by $P_{\mathcal{M}}$ the orthogonal projector in $\mathcal{K}^2$ to $\mathcal{M}$. A metric on $\mathrm{Gr}(2d, n)$ is defined by

$$d_n(\mathcal{M}_1, \mathcal{M}_2) := \|P_{\mathcal{M}_1} - P_{\mathcal{M}_2}\|.$$

Lemma 10.1. *Let $\mathcal{M} \subset \mathcal{K}^2$ with $\dim \mathcal{M} = n$, and let $\mathcal{M}_l \subset \mathcal{K}^2$, $l \in \mathbb{N}$, be a sequence of n-dimensional subspaces with*

$$\lim_{l \to \infty} d_n(\mathcal{M}_l, \mathcal{M}) = 0.$$

Then the sequence of operators $-\Delta(\mathcal{M}_l)$ converges in the strong graph limit to $-\Delta(\mathcal{M})$.

Proof. Denote by $\Gamma_{\mathcal{M}} \subset \mathcal{H}^2$ the graph of the operator $-\Delta(\mathcal{M})$ for arbitrary $\mathcal{M} \subset \mathcal{K}^2$. In order to prove convergence of $-\Delta(\mathcal{M}_l)$ to $-\Delta(\mathcal{M})$ in the strong graph limit (see [42, Sec. VIII.7, p. 293] for the definition), one has to prove two items:

1. For all $(\psi_l, -\Delta(\mathcal{M}_l)\psi_l) \in \mathcal{H}^2$, with $\psi_l \in \Delta(\mathcal{M}_l)$ such that $\psi_l \to \xi$ and $-\Delta(\mathcal{M}_l)\psi_l \to \eta$, it follows that $(\xi, \eta) \in \Gamma_{\mathcal{M}}$. This means $\xi \in \mathsf{D}(-\Delta(\mathcal{M}))$ and $\eta = -\Delta(\mathcal{M})\xi$.
2. For all $(\psi, -\Delta(\mathcal{M})\psi) \in \Gamma_{\mathcal{M}}$ there exists a sequence $\{\psi_l\}_{l \in \mathbb{N}}$ such that $(\psi_l, -\Delta(\mathcal{M}_l)\psi_l) \in \Gamma_{\mathcal{M}_l}$ and $\psi_l \to \psi$, $-\Delta(\mathcal{M}_l)\psi_l \to -\Delta(\mathcal{M})\psi$.

Note that $-\Delta(\mathcal{M})$ is an extension of finite rank of $-\Delta^0$ for any $\mathcal{M} \subset \mathcal{K}^2$. In particular, $\mathcal{D}^0 \subset \mathcal{D}$ is a closed subspace and the quotient space $\mathcal{D}/\mathcal{D}^0$ can be identified with the space of boundary values $\mathcal{K}^2$. Hence one has

$$\mathcal{D} = \mathcal{D}^0 \dot{+} \mathcal{K}^2, \tag{10.12}$$

where $\dot{+}$ denotes the direct sum. Let $\psi_l \to \xi$ and $-\Delta(\mathcal{M}_l)\psi_l \to \eta$. Since $-\Delta$ is closed and $-\Delta(\mathcal{M}_l)\psi_l = -\Delta\psi_l$ it follows that $\eta = -\xi''$. By (10.12) one has a decomposition

$$\xi = \xi^0 \dot{+} [\xi] \quad \text{and} \quad \psi_l = \psi_l^0 \dot{+} [\psi_l] \qquad \text{with } \xi^0, \psi_l^0 \in \mathcal{D}^0.$$

By assumption one has $\psi_l \to \xi$ in the graph norm which is equivalent to the Sobolev norm in the Hilbert space $\mathcal{D}$. Hence, $[\psi_l] \to [\xi]$ and therefore $\xi \in \mathsf{D}(-\Delta(\mathcal{M}))$ which proves (1).

Let $\psi \in \mathsf{D}(-\Delta(\mathcal{M}))$. Then by (10.12) one has the decomposition $\psi = \psi^0 \dot{+} [\psi]$. By assumption there is a sequence $[\psi_l] \to [\psi]$, and

$$\psi_l = \psi^0 \dot{+} [\psi_l] \in \mathsf{D}(-\Delta(\mathcal{M}_l)) \quad \text{such that } \psi_l \to \psi \quad \text{and } \psi_l'' \to \psi''.$$

This proves (2) and finishes the proof. □

Theorem 10.1. *Let A, B define irregular boundary conditions. Then there is a sequence of regular boundary conditions A_l, B_l, $l \in \mathbb{N}$, such that $-\Delta(A_l, B_l)$ converges in the strong graph limit to $-\Delta(A, B)$.*

Proof. For $\mathcal{M}(A,B) \subset \mathcal{K}^2$ with $\dim \mathcal{M}(A,B) = d$ one has by [27, Lem. 3.2]

$$P_{\mathcal{M}(A,B)^\perp} = \begin{pmatrix} A^* \\ B^* \end{pmatrix} (AA^* + BB^*)^{-1}(A,\, B). \tag{10.13}$$

Denote by P the orthogonal projector in $\mathcal{K}$ onto $\mathsf{N}B$. Then A and B_ϵ with

$$B_\epsilon := B + \epsilon P$$

define regular boundary conditions for $\epsilon > 0$ because B_ϵ is invertible. Note that by [27, Lem. 3.2] $AA^* + B_\epsilon B_\epsilon^*$, $\epsilon \geq 0$, is invertible since $\dim \mathcal{M}(A, B_\epsilon) = d$, and therefore

$$\lim_{\epsilon \to 0} (AA^* + B_\epsilon B_\epsilon^*)^{-1} = (AA^* + BB^*)^{-1}.$$

Using that $P_{\mathcal{M}(A,B_\epsilon)} = \mathbb{1} - P_{\mathcal{M}(A,B)^\perp}$, $\epsilon \geq 0$, and (10.13) one can prove then that

$$\lim_{\epsilon \to 0} \| P_{\mathcal{M}(A,B)} - P_{\mathcal{M}(A,B_\epsilon)} \| = 0,$$

where the norm is the operator norm, but since in the finite dimensional Hilbert space $\mathcal{K}^2$ all norms are equivalent it is also sufficient to prove component wise convergence. Applying Lemma 10.1 to $-\Delta(A,B)$ and to $-\Delta(A, B_{1/l})$, $l \in \mathbb{N}$, proves the claim. □

One has to emphasise that convergence in the strong graph limit does not imply convergence of spectra. Consider for example the operators $-\Delta(A_\tau, B_\tau)$ defined in Example 10.5. These operators converge for $\tau \to \pi/2$ in the strong graph limit to the operator $-\Delta(A_{\pi/2}, B_{\pi/2})$, which has empty resolvent set, whereas $-\Delta(A_\tau, B_\tau)$ for $\tau \neq \pi/2$ are similar to the self-adjoint Laplacian on the real line with spectrum $[0, \infty)$. The strong graph convergence for this special example was studied previously in [44, Prop. 2.7].

The approximation of regular boundary conditions in the norm resolvent sense will be established in Subsection 10.4.6.

10.3.9 $\mathcal{J}$-self-adjointness

Let $\mathcal{J} \colon \mathcal{H} \to \mathcal{H}$ be an anti-linear bounded operator with bounded inverse. The operator $\Delta(\mathcal{M})$ is called *$\mathcal{J}$-self-adjoint* if

$$\Delta(\mathcal{M})^* = \mathcal{J}^{-1} \Delta(\mathcal{M}) \mathcal{J}.$$

If $\mathcal{J}$ is in addition involutive and isometric, then our definition agrees with the standard notion from [14, Sec. III.5]. The usage of the $\mathcal{J}$-self-adjointness was suggested in [11] as a generalised concept of $\mathcal{PT}$-symmetry. It was also pointed out there that the residual spectrum of $\mathcal{J}$-self-adjoint operators is empty. The latter can be easily seen as follows, also for our broader definition. The equality $\Delta(\mathcal{M})^* - \lambda = \mathcal{J}^{-1} \left(\Delta(\mathcal{M}) - \overline{\lambda} \right) \mathcal{J}$ implies the symmetry relation $\overline{\sigma_{\mathrm{p}}(\Delta(\mathcal{M}))} = \sigma_{\mathrm{p}}(\Delta(\mathcal{M})^*)$. Using the general characterisation of the residual spectrum

$$\sigma_{\mathrm{r}}(-\Delta(\mathcal{M})) = \{ \lambda \notin \sigma_{\mathrm{p}}(-\Delta(\mathcal{M})) \mid \overline{\lambda} \in \sigma_{\mathrm{p}}(-\Delta(\mathcal{M})^*) \}, \tag{10.14}$$

it thus follows that the residual spectrum of $\Delta(\mathcal{M})$ is empty.

Let us further assume that $\mathcal{J}$ commutes with the maximal operator Δ, then $\mathcal{J}$ induces by

$$\underline{\mathcal{J}} \colon \mathcal{K} \to \mathcal{K}, \quad \underline{\psi} \mapsto \underline{\mathcal{J}\psi}$$

an anti-linear operator in $\mathcal{K}$, because the map $\psi \mapsto \underline{\psi}$ is surjective as a map from $\mathcal{W}$ to $\mathcal{K}$.

Proposition 10.4. *Let* $\dim \mathcal{M} = d$ *and* $\mathcal{M} = \mathcal{M}(A,B)$ *be such that* $A - \kappa B$ *is invertible for a* $\kappa > 0$. *Then* $\Delta(\mathcal{M})^*$ *is $\mathcal{J}$-self-adjoint if and only if* $\mathfrak{S}(i\kappa, A, B)$ *is $\underline{\mathcal{J}}$-self-adjoint,* i.e.,

$$\mathfrak{S}(i\kappa, A, B)^* = \underline{\mathcal{J}}^{-1}\, \mathfrak{S}(i\kappa, A, B) \underline{\mathcal{J}}.$$

Proof. It is sufficient to prove that $\mathcal{J}\colon \mathsf{D}(\Delta(\mathcal{M})^*) \to \mathsf{D}(\Delta(\mathcal{M}))$ is bijective. This is equivalent to $[\mathcal{J}]\mathcal{M}^* = \mathcal{M}$, where $\Delta(\mathcal{M})^* = \Delta(\mathcal{M}^*)$ and

$$[\mathcal{J}]\colon \mathcal{K}^2 \to \mathcal{K}^2, \quad \underline{\psi} \oplus \underline{\psi}' \mapsto \underline{\mathcal{J}\psi} \oplus \underline{(\mathcal{J}\psi)}'.$$

Let $[\psi] = \underline{\psi} \oplus \underline{\psi}' \in \mathcal{M}^*$, then by Proposition 10.3

$$-\frac{1}{2}\left(\mathfrak{S}(i\kappa, A, B)^* - \mathbb{1}\right)\underline{\psi} - \frac{1}{2\kappa}\left(\mathfrak{S}(i\kappa, A, B)^* + \mathbb{1}\right)\underline{\psi}' = 0,$$

and $[\mathcal{J}][\psi] \in \mathcal{M}$ if and only if

$$-\frac{1}{2}\left(\mathfrak{S}(i\kappa, A, B) - \mathbb{1}\right)\underline{\mathcal{J}\psi} - \frac{1}{2\kappa}\left(\mathfrak{S}(i\kappa, A, B) + \mathbb{1}\right)\underline{(\mathcal{J}\psi)'} = 0.$$

After applying $\underline{\mathcal{J}}^{-1}$, this is equivalent to

$$-\frac{1}{2}\left(\underline{\mathcal{J}}^{-1}\mathfrak{S}(i\kappa, A, B)\underline{\mathcal{J}} - \mathbb{1}\right)\underline{\psi} - \frac{1}{2\kappa}\left(\underline{\mathcal{J}}^{-1}\mathfrak{S}(i\kappa, A, B)\underline{\mathcal{J}} + \mathbb{1}\right)\underline{\psi}' = 0.$$

Therefore $[\mathcal{J}]\mathcal{M}^* = \mathcal{M}$ if and only if $\mathfrak{S}(i\kappa, A, B)^* = \underline{\mathcal{J}}^{-1}\mathfrak{S}(i\kappa, A, B)\underline{\mathcal{J}}$. □

An example for $\mathcal{J}$ being in addition involutive and isometric is the operator of complex conjugation

$$\mathcal{T}\colon \mathcal{H} \to \mathcal{H}, \quad \psi \mapsto \overline{\psi}.$$

In quantum mechanics, $\mathcal{T}$ has the physical meaning of the time-reversion operator. We remark that the time-reversion in quantum mechanics can be more complicated in spinorial models and it can be non-involutive, *cf* for instance [22], where Pauli equation is discussed. The origin of non-involutivity is the non-trivial action of $\mathcal{J}$ on the spinor components. The similar structure of $\mathcal{J}$ can be considered in the graph case as well, *e.g.* the composition of $\mathcal{T}$ and permutation of edges.

Corollary 10.3. *Let* $\dim \mathcal{M} = d$ *and* $\mathcal{M} = \mathcal{M}(A, B)$ *such that* $A - \kappa B$ *is invertible for a* $\kappa > 0$. *Then* $\Delta(\mathcal{M})^*$ *is* $\mathcal{T}$*-self-adjoint if and only if*

$$\mathfrak{S}(i\kappa, A, B)^* = \overline{\mathfrak{S}(i\kappa, A, B)}.$$

Example 10.7 (Complex δ-interactions are $\mathcal{T}$-self-adjoint)**.** Consider a finite metric graph and at each vertex $v \in \mathcal{V}$ impose complex δ-interactions with coupling constant $\gamma_v \in \mathbb{C}$. These are m-sectorial boundary conditions which can be parametrised at each vertex $v \in \mathcal{V}$ by a projector P_v and a rank one operator $L_v = -\frac{\gamma_v}{\deg(v)} P_v^{\perp}$, *cf* Example 10.4. Hence, at each vertex

$$\begin{aligned}\mathfrak{S}(k, A_v, B_v) &= -\left(L_v + P_v + ikP_v^{\perp}\right)^{-1}\left(L_v + P_v - ikP_v^{\perp}\right)\\ &= \left(-\frac{\gamma_v}{\deg(v)} + ik\right)^{-1}\left(\frac{\gamma_v}{\deg(v)} + ik\right)P_v^{\perp} + P_v.\end{aligned}$$

Consequently,

$$\mathfrak{S}(i\kappa, A_v, B_v)^* = \overline{\mathfrak{S}(i\kappa, A_v, B_v)},$$

for all $\kappa > 0$ such that $\frac{\gamma_v}{\deg(v)} + \kappa \neq 0$. Since

$$\mathfrak{S}(i\kappa, A, B) = \bigoplus_{v\in V} \mathfrak{S}(i\kappa, A_v, B_v),$$

where

$$A = \bigoplus_{v\in V} A_v \quad \text{and } B = \bigoplus_{v\in V} B_v,$$

the operator $-\Delta(A, B)$ defined by δ-interactions at each vertex is $\mathcal{T}$-self-adjoint for any complex coupling parameters, whereas it is self-adjoint only for real coupling parameters, *cf* [34, Sec. 3.2.1].

10.4 General spectral properties

In this section we collect some basic facts about the spectrum of the Laplacians on metric graphs.

10.4.1 Non-zero eigenvalues

A fundamental system of the equation $-\psi_k'' - k^2\psi_k = 0$ with $k \neq 0$ is given by the functions e^{ikx} and e^{-ikx}. For $\Im k > 0$ only the first of the mentioned functions is square integrable on the half line $[0,\infty)$ and hence on the external edges. Consequently, an *Ansatz* for an eigenfunction corresponding to an eigenvalue k^2 satisfying $\Im k > 0$ is to consider

$$\psi_k(x_j) = \begin{cases} s_j(k)e^{ikx_j}, & j \in \mathcal{E}, \\ \alpha_j(k)e^{ikx_j} + \beta_j(k)e^{-ikx_j}, & j \in \mathcal{I}. \end{cases}$$

The function ψ_k has the traces

$$\underline{\psi_k} = X(k;\underline{a}) \begin{bmatrix} \{s_j(k)\}_{j\in\mathcal{E}} \\ \{\alpha_j(k)\}_{j\in\mathcal{I}} \\ \{\beta_j(k)\}_{j\in\mathcal{I}} \end{bmatrix}, \qquad \underline{\psi_k'} = ik\cdot Y(k;\underline{a}) \begin{bmatrix} \{s_j(k)\}_{j\in\mathcal{E}} \\ \{\alpha_j(k)\}_{j\in\mathcal{I}} \\ \{\beta_j(k)\}_{j\in\mathcal{I}} \end{bmatrix},$$

where

$$X(k;\underline{a}) = \begin{bmatrix} \mathbb{1} & 0 & 0 \\ 0 & \mathbb{1} & \mathbb{1} \\ 0 & e^{ik\underline{a}} & e^{-ik\underline{a}} \end{bmatrix} \quad \text{and} \quad Y(k;\underline{a}) = \begin{bmatrix} \mathbb{1} & 0 & 0 \\ 0 & \mathbb{1} & -\mathbb{1} \\ 0 & -e^{ik\underline{a}} & e^{-ik\underline{a}} \end{bmatrix}$$

are given with respect to the decomposition $\mathcal{K} = \mathcal{K}_{\mathcal{E}} \oplus \mathcal{K}_{\mathcal{I}}^- \oplus \mathcal{K}_{\mathcal{I}}^+$. Here $e^{\pm ik\underline{a}}$ denote $(|\mathcal{I}|\times|\mathcal{I}|)$-diagonal matrices with entries $\{e^{\pm ik\underline{a}}\}_{i,j} = \delta_{i,j}e^{\pm ika_i}$.

The function ψ_k is an eigenfunction to the eigenvalue k^2 if and only if $\psi_k \in \mathsf{D}(-\Delta(A,B))$. This is the case if and only if the *Ansatz* function ψ_k satisfies the boundary conditions, which are encoded in the equation

$$Z(k;A,B,\underline{a}) \begin{bmatrix} \{s_j(k)\}_{j\in\mathcal{E}} \\ \{\alpha_j(k)\}_{j\in\mathcal{I}} \\ \{\beta_j(k)\}_{j\in\mathcal{I}} \end{bmatrix} = 0,$$

where

$$Z(k;A,B,\underline{a}) = AX(k;\underline{a}) + ik\,BY(k;\underline{a}).$$

Hence k^2 with $\Im k > 0$ is an eigenvalue of $\Delta(A,B)$ if and only if

$$\det Z(k;A,B,\underline{a}) = 0, \tag{10.15}$$

and k^2 has geometric multiplicity $\dim \mathsf{N}Z(k;A,B,\underline{a})$.

For $\mathcal{E} = \emptyset$ the solutions of $\det Z(k;A,B,\underline{a}) = 0$ for $k > 0$ are also eigenvalues, whereas for $\mathcal{I} = \emptyset$ the solutions of $\det Z(k;A,B,\underline{a}) = 0$ for $k > 0$ are not eigenvalues. In particular, for $\mathcal{I} = \emptyset$ there are no positive real eigenvalues since neither e^{ikx} nor e^{-ikx} is square integrable on the half-line and therefore on the external edges. This is illustrated by the following example.

Example 10.8 (Graph with a spectral singularity)**.** Consider the graph consisting of only one half-line, that is $|\mathcal{E}| = 1$ and $\mathcal{I} = \emptyset$, and impose the non-self-adjoint regular boundary conditions defined by $A = -i$ and $B = 1$, *i.e.* $-i\psi(0) + \psi'(0) = 0$. Then $k = 1$ is a solution of $\det(A + ikB) = 0$, but $k^2 = 1$ is not an eigenvalue of $-\Delta(A,B)$. In [16, Ex. 3] it is shown that 1 is in the continuous spectrum, but it is a spectral singularity, which means that the limits

$$\lim_{\epsilon\to 0+} \int_I \left[(-\Delta(A,B) - \lambda + \epsilon)^{-1} - (-\Delta(A,B) - \lambda - \epsilon)^{-1}\right] d\lambda,$$

where I are some bounded real intervals, are singular in a certain sense; see [16, Def. 1] for the precise definition and for further references on the topic. An alternative definition of spectral singularities is related to the limit of the resolvent kernel when approaching non-isolated points in the spectrum [16, Def. 4]. This phenomenon will be discussed further in Remark 10.6 below, after giving an explicit expression for the resolvent kernel in Proposition 10.7.

For self-adjoint boundary conditions it is known that all solutions of (10.15) for $k > 0$ are eigenvalues [23, Thm. 3.1], including the cases $\mathcal{E} \neq \emptyset$ and $\mathcal{I} \neq \emptyset$. However, for non-self-adjoint boundary conditions this is not true anymore and it is difficult to study the positive real eigenvalues when $\mathcal{E} \neq \emptyset$ and $\mathcal{I} \neq \emptyset$. These eigenvalues are embedded in the essential spectrum as shown below in Subsection 10.4.7.

Remark 10.2. The function $k \mapsto \det Z(k;A,B,\underline{a})$ is holomorphic on the whole complex plain, hence it either vanishes identically or its zeros form a discrete set. Consequently one has for $\dim \mathcal{M}(A,B) \geq d$ that $\operatorname{clo}\sigma_{\mathrm{p}}(-\Delta(A,B))$ is either entire $\mathbb{C}$ or at most discrete, where clo denotes the closure in $\mathbb{C}$.

10.4.2 Eigenvalue zero

Eigenfunctions to the eigenvalue zero are piecewise affine, because a fundamental system of the equation $\psi'' = 0$ is given by the constant solution and the linear solution. This gives the *Ansatz*

$$\psi_0(x_j) = \begin{cases} 0, & j \in \mathcal{E}, \\ \alpha_j^0 + \beta_j^0 x_j, & j \in \mathcal{I}, \end{cases}$$

with traces

$$\underline{\psi_0} = X_0\,(\underline{a}) \begin{bmatrix} 0 \\ \{\alpha_j^0\}_{j\in\mathcal{I}} \\ \{\beta_j^0\}_{j\in\mathcal{I}} \end{bmatrix}, \qquad \underline{\psi_0'} = Y_0\,(\underline{a}) \begin{bmatrix} 0 \\ \{\alpha_j^0\}_{j\in\mathcal{I}} \\ \{\beta_j^0\}_{j\in\mathcal{I}} \end{bmatrix},$$

where

$$X_0\,(\underline{a}) = \begin{bmatrix} 0 & 0 & 0 \\ 0 & \mathbb{1} & 0 \\ 0 & \mathbb{1} & \underline{a} \end{bmatrix} \quad \text{and} \quad Y_0\,(\underline{a}) = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & \mathbb{1} \\ 0 & 0 & -\mathbb{1} \end{bmatrix}.$$

Consequently zero is an eigenvalue of the operator $-\Delta(A, B)$ if and only if there are α_j^0, β_j^0, with $j \in \mathcal{I}$, such that

$$[AX_0\,(\underline{a}) + BY_0\,(\underline{a})] \begin{bmatrix} 0 \\ \{\alpha_j^0\}_{j\in\mathcal{I}} \\ \{\beta_j^0\}_{j\in\mathcal{I}} \end{bmatrix} = 0$$

has a non-trivial solution. For $\mathcal{E} = \emptyset$ zero is an eigenvalue if and only if

$$\det\left(AX_0(\underline{a}) + BY_0(\underline{a})\right) = 0,$$

and for $\mathcal{I} = \emptyset$ zero cannot be an eigenvalue.

10.4.3 Operators with empty resolvent set

For non-self-adjoint Laplacians the resolvent set is not always non-empty, and one needs a certain number of boundary conditions to define operators of which the spectrum forms a proper subset of $\mathbb{C}$.

Proposition 10.5. *Let* $\dim \mathcal{M} \neq d$*, then* $\sigma(\Delta(\mathcal{M})) = \mathbb{C}$*. In particular, if* $\dim \mathcal{M} > d$ *then* $\operatorname{clo} \sigma_{\mathrm{p}}(\Delta(\mathcal{M})) = \mathbb{C}$*, where* clo *denotes the closure in* $\mathbb{C}$*.*

Proof. For $\mathcal{M}$ with $\dim \mathcal{M} > d$ there are maps A, B in $\mathcal{K}$ such that $\mathcal{M} = \mathcal{M}(A, B)$. By assumption the map $(A,\ B)$ is not surjective, and therefore also

$$Z\,(k; \underline{a}, A, B) = (A,\ B) \circ \begin{pmatrix} X(k; \underline{a}) \\ ik\,Y(k; \underline{a}) \end{pmatrix}$$

is not surjective for any k. Consequently $\det Z\,(k; \underline{a}, A, B) = 0$ for all $k \in \mathbb{C}$ which proves that $\mathbb{C} \setminus [0, \infty) \subset \sigma_{\mathrm{p}}(-\Delta(A, B))$. Since the spectrum is a closed set, we conclude with $\sigma(\Delta(A, B)) = \mathbb{C}$.

Let $\dim \mathcal{M} < d$. Then, by Corollary 10.1, $\dim \mathcal{M}^* > d$, and hence $\sigma(\Delta(\mathcal{M})^*) = \mathbb{C}$. Since $\sigma(\Delta(\mathcal{M})) = \overline{\sigma(\Delta(\mathcal{M})^*)}$, *cf* [20, Thm. III.6.22], the claim follows. □

As already discussed for irregular boundary conditions defined by A, B, the resolvent set can be empty even if $\dim \mathcal{M}(A, B) = d$, *cf* Example 10.1.

10.4.4 Residual spectrum for regular boundary conditions

Following [24, Eq. (3.7)], for regular boundary conditions with $A + ikB$ invertible the secular equation (10.15) can be rewritten using the identity

$$Z\,(k; A, B, \underline{a}) = (A + ikB)\,[\mathbb{1} - \mathfrak{S}(k, A, B) T(k; \underline{a})]\, R_+(k; \underline{a}), \tag{10.16}$$

where

$$T(k; \underline{a}) = \begin{bmatrix} 0 & 0 & 0 \\ 0 & 0 & e^{ik\underline{a}} \\ 0 & e^{ik\underline{a}} & 0 \end{bmatrix} \quad \text{and} \quad R_+(k, \underline{a}) = \begin{bmatrix} \mathbb{1} & 0 & 0 \\ 0 & \mathbb{1} & 0 \\ 0 & 0 & e^{-ik\underline{a}} \end{bmatrix}.$$

In particular one obtains

Lemma 10.2. *Let A, B define regular boundary conditions. Then*

$$\operatorname{clo}\sigma_{\mathrm{p}}(-\Delta(A,B)) \neq \mathbb{C},$$

and $\lambda \in \sigma_{\mathrm{p}}(-\Delta(A,B)) \setminus [0,\infty)$ if and only if $\overline{\lambda} \in \sigma_{\mathrm{p}}(-\Delta(A,B)^*) \setminus [0,\infty)$.

Proof. For A, B defining regular boundary conditions $\mathfrak{S}(i\kappa, A, B)$ is defined for every $\kappa > 0$ except a finite set and $\mathbb{1} - \mathfrak{S}(i\kappa, A, B)T(i\kappa; \underline{a})$ is invertible for κ large enough and the first claim follows from (10.16).

To prove the second claim, we first notice that for $A \pm ikB$ invertible one has with (10.16)

$$\begin{aligned} &Z\,(k; A, B, \underline{a}) \\ &\qquad = (A + ikB)\,[\mathbb{1} - \mathfrak{S}(k, A, B)T(k; \underline{a})]\,\mathfrak{S}(k, A, B)\mathfrak{S}(k, A, B)^{-1}R_+(k; \underline{a}). \end{aligned}$$

Since $Z\,(k; A, B, \underline{a})$ is holomorphic in entire $\mathbb{C}$ the above representation admits continuous continuation to $\mathbb{C}$. So, taking the adjoint one obtains

$$\overline{\det Z\,(k; A, B, \underline{a})} = \det(A^* - i\overline{k}B^*) \det\left[\mathbb{1} - \mathfrak{S}(k, A, B)^* T(-\overline{k}; \underline{a})\right] \det R_+(-\overline{k}; \underline{a})$$

for all $k \in \mathbb{C}$ except a finite set, where one has used

$$\begin{aligned} &\det\Big([\mathfrak{S}(k, A, B)^*]^{-1}\,\mathfrak{S}(k, A, B)^*\,[\mathbb{1} - T(k; \underline{a})^*\mathfrak{S}(k, A, B)^*]\Big) \\ &\qquad\qquad = \det\left[\mathbb{1} - \mathfrak{S}(k, A, B)^* T(-\overline{k}; \underline{a})\right]. \end{aligned}$$

Applying Proposition 10.3 and choosing the representation $A_{\mathfrak{S}}, B_{\mathfrak{S}}$ given there, we arrive at

$$\mathfrak{S}(k, A, B)^* = \mathfrak{S}(-\overline{k}, A', B')$$

and hence

$$\overline{\det Z\,(k; A, B, \underline{a})} = \det Z\left(-\overline{k}; A', B', \underline{a}\right)$$

for all $k \in \mathbb{C}$ except a finite set. By continuous continuation the claim follows for all $k \in \mathbb{C}$, and hence k^2, $\Im k > 0$, is an eigenvalue of $-\Delta(A, B)$ if and only if $\overline{k}^2$ is an eigenvalue of $-\Delta(A, B)^*$. □

Remark 10.3. Note that for $\mathcal{E} = \emptyset$ one can even show that $\lambda \in \sigma_{\mathrm{p}}(-\Delta(A,B))$ if and only if $\overline{\lambda} \in \sigma_{\mathrm{p}}(-\Delta(A,B)^*)$.

Remark 10.4 (Stability of eigenvalues under similarity of scattering matrices)**.** Let $(\mathcal{G}, \underline{a})$ be a compact finite metric graphs. Let A, B and A', B' define regular boundary conditions, and assume that there is an invertible map $G(k)$, $k \in \mathbb{C}$, such that

$$\mathfrak{S}(k, A, B) = G(k)^{-1}\mathfrak{S}(k, A', B')G(k) \quad \text{and} \quad G(k)T(k; \underline{a}) = T(k; \underline{a})G(k),$$

for all $k \in \mathbb{C}$. Then using (10.16) and one obtains immediately

$$\sigma_{\mathrm{p}}(-\Delta(A, B)) = \sigma_{\mathrm{p}}(-\Delta(A', B'))$$

and the geometric multiplicity of the eigenvalues agrees.

Combining Lemma 10.2 with the general characterisation of the residual spectrum (10.14), we obtain the following useful property.

Proposition 10.6. *Let A, B define regular boundary conditions then the residual spectrum $\sigma_{\mathrm{r}}(-\Delta(A,B))$ is contained in $[0,\infty)$. If $\mathcal{E} = \emptyset$ or $\mathcal{I} = \emptyset$ then $\sigma_{\mathrm{r}}(-\Delta(A,B)) = \emptyset$.*

In particular, using (10.14) and Remark 10.2 it follows that the residual spectrum forms a discrete subset of $[0,\infty)$. That the residual spectrum is in general not empty is shown by the following example.

Example 10.9 (Graph with a residual spectrum)**.** Consider the metric graph consisting of one internal edge of length a and one external edge. Impose the following boundary conditions

$$\psi'_{\mathcal{E}}(0) = 0, \quad -i\psi_{\mathcal{I}}(0) + \psi'_{\mathcal{I}}(0) = 0, \quad \psi_{\mathcal{E}}(0) + i\psi_{\mathcal{I}}(a) - \psi'_{\mathcal{I}}(a) = 0.$$

These are m-sectorial boundary conditions with

$$P = 0 \quad \text{and} \quad L = \begin{bmatrix} 0 & 0 & 0 \\ 0 & -i & 0 \\ 1 & 0 & i \end{bmatrix}.$$

A direct computation shows that

$$\psi(x) = \begin{cases} 0, & x \in \mathcal{E}, \\ e^{ix}, & x \in \mathcal{I}, \end{cases}$$

is an eigenfunction of $-\Delta(L, \mathbb{1})$ corresponding to the eigenvalue 1. By Corollary 10.2 the adjoint operator is given by $-\Delta(L^*, \mathbb{1})$, which is defined by the boundary conditions

$$\psi_{\mathcal{I}}(a) + \psi'_{\mathcal{E}}(0) = 0, \quad i\psi_{\mathcal{I}}(0) + \psi'_{\mathcal{I}}(0) = 0, \quad i\psi_{\mathcal{I}}(a) + \psi'_{\mathcal{I}}(a) = 0.$$

For the second condition an eigenfunction corresponding to the eigenvalue 1 would be e^{-ix} on the internal edge and for the square integrability 0 on the external edge, but this function does not satisfy the third boundary condition nor the first. Therefore 1 is an eigenvalue of $-\Delta(L, \mathbb{1})$, but not an eigenvalue of $-\Delta(L^*, \mathbb{1})$. Using the characterisation of the residual spectrum in (10.14), one obtains that $1 \in \sigma_{\mathrm{r}}(-\Delta(L^*, \mathbb{1}))$.

10.4.5 Resolvents for regular boundary conditions

In [27, Lem. 3.10] an explicit formula for the resolvent associated with $k^2 \in \rho(-\Delta(A, B))$ is given. In this subsection we reproduce the result for regular boundary conditions and add a criterion for k^2 being in the resolvent set. Since the result of [27, Lem. 3.10] is given without proof (arguing that it can be proved "in the exactly the same way" as for self-adjoint boundary conditions), we provide a short proof in the appendix (where we also recall the notion of integral operators, *cf* Definition 10.3). This will make our paper self-consistent and, moreover, clarify the need for regularity of boundary conditions in the proof.

Proposition 10.7. *Let A, B define regular boundary conditions such that*

$$A \pm ikB \quad \textit{and} \quad \mathbb{1} - \mathfrak{S}(k, A, B)T(k; \underline{a})$$

are invertible for $k \in \mathbb{C}$ with $\Im k > 0$. Then $k^2 \in \rho(-\Delta(A, B))$ and the resolvent $\left(-\Delta(A, B) - k^2\right)^{-1}$ is the integral operator with the $(|\mathcal{E}| + |\mathcal{I}|) \times (|\mathcal{E}| + |\mathcal{I}|)$ matrix valued integral kernel $r_{\mathcal{M}}(x, y; k)$, $\mathcal{M} = \mathcal{M}(A, B)$, admitting the representation

$$r_{\mathcal{M}}(x, y; k) = r^0(x, y; k) + r^1_{\mathcal{M}}(x, y; k)$$

with $\{r^0(x, y; k)\}_{j,j'} = \delta_{j,j'} \frac{i}{2k} e^{ik|x_j - y_j|}$ and

$$r^1_{\mathcal{M}}(x, y; k) = \frac{i}{2k} \Phi(x, k) R_+(k; \underline{a})^{-1} \left[\mathbb{1} - \mathfrak{S}(k, A, B)T(k; \underline{a})\right]^{-1} \mathfrak{S}(k, A, B) R_+(k; \underline{a})^{-1} \Phi(y, k)^T,$$

where the matrix $\Phi(x, k)$ is given by

$$\Phi(x, k) := \begin{bmatrix} \phi(x, k) & 0 & 0 \\ 0 & \phi_+(x, k) & \phi_-(x, k) \end{bmatrix}$$

with diagonal matrices $\phi(x, k) = \mathrm{diag}\{e^{ikx_j}\}_{j \in \mathcal{E}}$ and $\phi_\pm(x, k) = \mathrm{diag}\{e^{\pm ikx_j}\}_{j \in \mathcal{I}}$, and $\Phi(x, k)^T$ denotes the transposed of $\Phi(x, k)$.

Remark 10.5. The statement of the proposition holds also for $k > 0$ if $\mathcal{E} = \emptyset$.

Remark 10.6. Note that the resolvent kernel $r_{\mathcal{M}}(x, y, k)$ is still well-defined for $k > 0$ such that

$$A \pm ikB \quad \text{and} \quad \mathbb{1} - \mathfrak{S}(k, A, B)T(k; \underline{a})$$

are invertible. For these $k > 0$ the kernel $r_{\mathcal{M}}(x, y, k)$ still defines an operator from $L^2(\mathcal{G}, e^{x\delta} dx)$ to $L^2(\mathcal{G}, dx)$ for $\delta > 0$. In the sense of [16, Def. 4] the points $k^2 > 0$ such that $\lim_{\epsilon \to 0+} r_{\mathcal{M}}(x, y, k + i\epsilon)$, $k > 0$, is unbounded are called spectral singularities. Example 10.8 shows that the spectral singularities can form a larger set than the set of embedded eigenvalues.

10.4.6 Approximation of regular boundary conditions

Using the explicit formula for the resolvent, one can establish a norm resolvent convergence for certain regular boundary conditions.

Proposition 10.8. *Let A_ϵ, B_ϵ, $\epsilon \geq 0$, define regular boundary conditions such that*

$$A_\epsilon \pm ikB_\epsilon \quad \text{and} \quad \mathbb{1} - \mathfrak{S}(k, A_\epsilon, B_\epsilon)T(k; \underline{a})$$

are invertible for a certain $k \in \mathbb{C}$ with $\Im k > 0$ and all $\epsilon \geq 0$. Assume furthermore that

$$\lim_{\epsilon \to 0} \mathfrak{S}(k, A_\epsilon, B_\epsilon) = \mathfrak{S}(k, A_0, B_0).$$

Then $k^2 \in \rho(-\Delta(A_\epsilon, B_\epsilon))$ for all $\epsilon \geq 0$, and

$$\lim_{\epsilon \to 0} \left\| \left(-\Delta(A_\epsilon, B_\epsilon) - k^2\right)^{-1} - \left(-\Delta(A_0, B_0) - k^2\right)^{-1} \right\| = 0.$$

Proof. Set $\mathcal{M}_\epsilon := \mathcal{M}(A_\epsilon, B_\epsilon)$ for $\epsilon \geq 0$. Then

$$r_{\mathcal{M}_\epsilon}(x, y; k) - r_{\mathcal{M}_0}(x, y; k) = r^1_{\mathcal{M}_\epsilon}(x, y; k) - r^1_{\mathcal{M}_0}(x, y; k).$$

Note that $r^1_{\mathcal{M}_\epsilon}(\cdot, \cdot; k)$ define for every $\epsilon \geq 0$ Hilbert-Schmidt operators. One obtains

$$\begin{aligned} &\|r^1_{\mathcal{M}_\epsilon}(\cdot, \cdot; k) - r^1_{\mathcal{M}_0}(\cdot, \cdot; k)\|_{\mathrm{HS}} \\ &\qquad \leq \frac{C(k)}{2k} \Big\| \left[\mathbb{1} - \mathfrak{S}(k, A_\epsilon, B_\epsilon)T(k; \underline{a})\right]^{-1} \mathfrak{S}(k, A_\epsilon, B_\epsilon) \\ &\qquad\qquad - \left[\mathbb{1} - \mathfrak{S}(k, A_0, B_0)T(k; \underline{a})\right]^{-1} \mathfrak{S}(k, A_0, B_0) \Big\|, \end{aligned}$$

because $r(x, y; k) = \Phi(x, k)R_+(k; \underline{a})^{-2}\Phi(y, k)^T$ defines a Hilbert-Schmidt operator $R(k)$, with a finite Hilbert-Schmidt norm $\|r(\cdot, \cdot; k)\|_{\mathrm{HS}} =: C(k)$. From the convergence of $\mathfrak{S}(k, A_\epsilon, B_\epsilon)$ to $\mathfrak{S}(k, A_0, B_0)$ it follows under the assumptions imposed that

$$\lim_{\epsilon \to 0} \left[\mathbb{1} - \mathfrak{S}(k, A_\epsilon, B_\epsilon)T(k; \underline{a})\right]^{-1} = \left[\mathbb{1} - \mathfrak{S}(k, A_0, B_0)T(k; \underline{a})\right]^{-1}.$$

Hence,

$$\begin{aligned} 0 &\leq \lim_{\epsilon \to 0} \left\| \left(-\Delta(A_\epsilon, B_\epsilon) - k^2\right)^{-1} - \left(-\Delta(A_0, B_0) - k^2\right)^{-1} \right\| \\ &\leq \lim_{\epsilon \to 0} \left\| \left(-\Delta(A_\epsilon, B_\epsilon) - k^2\right)^{-1} - \left(-\Delta(A_0, B_0) - k^2\right)^{-1} \right\|_{\mathrm{HS}} = 0, \end{aligned}$$

which proves the claim. ☐

In contrast to the convergence in the strong graph sense established in Subsection 10.3.8, the norm resolvent convergence implies the convergence of spectra.

10.4.7 Essential spectra for regular boundary conditions

For non-self-adjoint operators there are various notions of the essential spectrum. Five types, defined in terms of Fredholm properties and denoted by $\sigma_{\mathrm{e}j}$ for $j = 1, 2, 3, 4, 5$, are in detail discussed in [14, Chap. IX]. All these essential spectra coincide for T self-adjoint, but for closed non-self-adjoint T one has in general only the inclusions $\sigma_{\mathrm{e}j}(T) \subset \sigma_{\mathrm{e}_i}(T)$ with $j < i$. The largest set $\sigma_{\mathrm{e}5}(T)$ is known as the essential spectrum due to Browder and it coincides with the complement in the spectrum of isolated eigenvalues λ of finite algebraic multiplicity such that $\mathsf{R}(T - \lambda)$ is closed.

Proposition 10.9. *Let A, B define through* (10.5) *regular boundary conditions. Then $\rho(-\Delta(A, B)) \neq \emptyset$. For $\mathcal{E} \neq \emptyset$ one has $\sigma_{\mathrm{e}5}(-\Delta(A, B)) = [0, \infty)$. For $\mathcal{E} = \emptyset$ the spectrum is purely discrete and the resolvent is compact, hence $\sigma_{\mathrm{e}5}(-\Delta(A, B)) = \emptyset$.*

Proof. From Lemma 10.2 together with Proposition 10.7 it follows that the resolvent set is not empty and that the resolvents for any regular boundary conditions differ only by a perturbation of finite rank. In particular, the difference of respective resolvents is compact.

Assume $\mathcal{E} \neq \emptyset$. Self-adjoint realisations are also defined by regular boundary conditions and it is well known that the essential spectrum is $[0, \infty)$ in this case. Applying the Weyl-type perturbation result from [14, Thm. IX.2.4], it follows that $\sigma_{\mathrm{e}i}(-\Delta(A, B)) = [0, \infty)$ with $i = 1, 2, 3, 4$. Since $\mathbb{C} \setminus \sigma_{\mathrm{e}1}(-\Delta(A, B))$ has only one connected component, which intersects the resolvent set of $-\Delta(A, B)$, $\sigma_{\mathrm{e}5}(-\Delta(A, B)) = \sigma_{\mathrm{e}1}(-\Delta(A, B))$ by the very definition of [14, Chap. IX].

Now let $\mathcal{E} = \emptyset$. Then all self-adjoint realisations have compact resolvent, Proposition 10.7 applies and the resolvents for any regular boundary conditions differ only by a perturbation of finite rank. Hence the resolvent is compact for all regular boundary conditions which proves the assertion. ☐

In particular, one obtains that on finite compact metric graphs for regular boundary conditions the spectrum is purely discrete, there is no continuous nor residual spectrum. For graphs with $\mathcal{I} = \emptyset$ there are at most finitely many eigenvalues in $\mathbb{C} \setminus [0, \infty)$, they have finite algebraic multiplicity, and the continuous spectrum is $[0, \infty)$, whereas the residual spectrum is empty. For the case $\mathcal{E} \neq \emptyset$ and $\mathcal{I} \neq \emptyset$ it is difficult to give general statements on eigenvalues and residual spectrum contained in $[0, \infty)$.

10.5 Riesz basis on compact graphs

In this section we apply a general result due to Agranovich [1] about a Riesz basis property to m-sectorial Laplacians on finite compact metric graphs. Throughout this section let us therefore assume that $(\mathcal{G}, \underline{a})$ is an arbitrary finite compact metric graph, *i.e.* $\mathcal{E} = \emptyset$.

Let us first recall the definition of the Riesz basis of subspaces; see, *e.g.*, [38] for more details. The set of subspaces $\{\mathcal{N}_k\}_{k=1}^{\infty} \subset \mathcal{H}$ is called a *basis of subspaces* if any vector f from the Hilbert space $\mathcal{H}$ can be uniquely represented as a series

$$f = \sum_{k=1}^{\infty} f_k, \qquad f_k \in \mathcal{N}_k.$$

Such a basis is called unconditional or *Riesz* if it remains a basis after any permutation of the subspaces appearing in it, *i.e.*, if the above series converges unconditionally for any f. If the subspaces are one dimensional, we obtain the standard notion of Riesz basis.

Let P be an orthogonal projector in $\mathcal{K}$, $P^{\perp} = \mathbb{1} - P$ its complementary projector and L a not necessarily self-adjoint operator in $\mathcal{K}$ with $L = P^{\perp} L P^{\perp}$. Then one considers $-\Delta(P + L, P^{\perp})$. Recall that this operator is associated with the closed sectorial form $\delta_{P,L}$ defined by (10.9). The main result of this section reads as follows.

Theorem 10.2. *The spectrum of the operator $-\Delta(P + L, P^{\perp})$ is purely discrete, and there is a Riesz basis consisting of finite dimensional invariant subspaces of $-\Delta(P + L, P^{\perp})$.*

The proof of Theorem 10.2 is based on the following abstract result due to Agranovich [1].

Theorem 10.3 ([1, Thm. in Sec. 1])**.** *Let $\mathcal{H}$ and $\mathcal{W} \subset \mathcal{H}$ be separable Hilbert spaces, where the imbedding $\mathcal{W} \hookrightarrow \mathcal{H}$ is compact. Consider a closed sectorial form $\mathfrak{a}$ with domain $\mathsf{D}\mathfrak{a} = \mathcal{W}$, and denote by A the m-sectorial operator defined by $\mathfrak{a}$. Assume that there are constants $c, C > 0$ such that*

$$c\,\|\psi\|_{\mathcal{W}}^2 \leq \Re\mathfrak{a}[\psi] \quad \text{for all } \psi \in \mathcal{W} \tag{10.17}$$

and

$$|\mathfrak{a}[\psi, \varphi]| + |(\Re\mathfrak{a})[\psi, \varphi]| \leq C \|\psi\|_{\mathcal{W}} \|\varphi\|_{\mathcal{W}} \quad \text{for all } \psi, \varphi \in \mathcal{W}, \tag{10.18}$$

where $\Re\mathfrak{a}$ denotes the real part of the form $\mathfrak{a}$. Let B be the operator defined by $\Re\mathfrak{a}$ and assume furthermore that for some $0 \leq q < 1$ and $\gamma > 0$

$$|\Im\mathfrak{a}[\psi]| \leq \gamma \|B^{1/2}\psi\|^{2q} \|\psi\|^{2-2q} \quad \text{for all } \psi \in \mathcal{W}, \tag{10.19}$$

where $\Im\mathfrak{a}$ denotes the imaginary part of $\mathfrak{a}$. Denote by $\lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_j \leq \ldots$ the eigenvalues of B (counting multiplicities) and assume that for some $p > 0$

$$\limsup_{j \to \infty} \lambda_j j^{-p} > 0. \tag{10.20}$$

Then there exists a Bari basis if $p(1-q) > 1$, a Riesz basis if $p(1-q) = 1$, and an Abel basis of order $\beta = \beta_0 + \beta_1$ if $p(1-q) < 1$, consisting of finite dimensional subspaces invariant with respect to A respectively. Here, $\beta_0 = p^{-1} - (1-q)$ and β_1 is an arbitrarily small positive number.

To apply Theorem 10.3, we need the following elementary inequality, which we state here without proof.

Lemma 10.3. *There exists a constant $C > 0$ such that for all $\psi \in W^{1,2}((0, a))$*

$$\|\psi\|_{L^\infty}^2 \leq C \|\psi\|_{\mathcal{W}} \|\psi\|.$$

Now we are in a position to prove Theorem 10.2.

Proof of Theorem 10.2. Consider the form $\mathfrak{a}' := \delta_{P,L}$ defined by (10.9). We apply Theorem 10.3 to the form $\mathfrak{a} := \mathfrak{a}' + \epsilon$ with an appropriate $\epsilon > 0$.

There is an $\epsilon > 0$ such that the form $\mathfrak{b} := \Re\mathfrak{a} + \epsilon > 0$ defines a norm that is equivalent to the Sobolev norm of $\mathcal{W}$. Indeed, using Lemma 10.3 together with Young's inequality, we have

$$\begin{aligned} -\langle \Re L\underline{\psi}, \underline{\psi}\rangle_{\mathcal{K}} &\geq -\|\Re L\|\,\|\underline{\psi}\|^2 \geq -C\|\psi\|_{\mathcal{W}}\|\psi\| \\ &\geq -\delta\|\psi\|^2_{\mathcal{W}} - \frac{C^2}{4\delta}\|\psi\|^2, \qquad \text{for any } \delta > 0. \end{aligned}$$

Hence, for $\delta < 1$ and $\epsilon > 0$ such that $\frac{C^2}{4\delta} < \epsilon$, one has

$$\int_{\mathcal{G}} |\psi'|^2 - \langle \Re L\underline{\psi}, \underline{\psi}\rangle + \epsilon\|\psi\|^2 \geq \gamma\|\psi\|^2_{\mathcal{W}},$$

where

$$\gamma = \min\left\{\epsilon - \frac{C^2}{4\delta}, 1 - \delta\right\}.$$

The other inequality can be shown analogously.

Using the notation of Theorem 10.3, we have

$$\begin{aligned} \Re\mathfrak{a}[\psi] &= \int_{\mathcal{G}} |\psi'|^2 - \langle \Re L P^\perp\underline{\psi}, P^\perp\underline{\psi}\rangle_{\mathcal{K}} + \epsilon\|\psi\|^2, \\ \Im\mathfrak{a}[\psi] &= -\langle \Im L P^\perp\underline{\psi}, P^\perp\underline{\psi}\rangle_{\mathcal{K}}, \end{aligned}$$

where

$$\mathsf{D}\mathfrak{a} = \mathsf{D}\Re\mathfrak{a} = \mathcal{W}_P := \{\psi \in \mathcal{W} \mid P\underline{\psi} = 0\} \subset \mathcal{H}.$$

The space $\mathcal{W}$ with the inner product $\langle\cdot,\cdot\rangle_{\mathcal{W}}$ is a Hilbert space and $\mathcal{W}_P$ is a closed subspace. Since $(\mathcal{G}, \underline{a})$ is compact, $\mathcal{W}_P$ is compactly embedded in $\mathcal{H}$. Condition (10.17) is fulfilled for $\Re\mathfrak{a}$ and Condition (10.18) follows as well by applying the Cauchy-Schwarz inequality. Recall that the norm defined by $\mathfrak{b}$ is equivalent to the Sobolev norm in the Hilbert space $\mathcal{W}_P$. Therefore, there is a constant $C > 0$ such that $\|\psi'\| \leq \|\psi\|_{\mathcal{W}} \leq C\|B^{1/2}\psi\| = C\mathfrak{b}[\psi]$. Applying Lemma 10.3 to the form $\Im\mathfrak{a}$ yields

$$|\Im\mathfrak{a}[\psi]| \leq \|\Im L\|\,\|\underline{\psi}\|^2_{\mathcal{K}} \leq C\|\psi\|\|\psi\|_{\mathcal{W}} \leq C\|\psi\|\|B^{1/2}\psi\|,$$

where $C > 0$ is used as universal constant. Thus Condition (10.19) is fulfilled with $q = 1/2$.

From [18, Thm. 3.1] it follows that the operator associated with $\mathfrak{b}$ is the self-adjoint operator $B = -\Delta(P + \Re L, P^\perp) + \epsilon$. Since its spectrum is discrete, there is a variational characterisation of the eigenvalues in terms of the minimax principle. Applying a Dirichlet-Neumann-bracketing one arrives at the conclusion that $\lambda_j = O(j^2)$, see, *e.g.*, [10, Prop. 4.2], and hence Condition (10.20) holds for $p = 2$.

Putting the pieces together, we obtain that Theorem 10.3 applies to $\mathfrak{a}$, which defines the operator $A = A' + \epsilon$, where $A' = -\Delta(P + L, P^\perp)$. Since the invariant subspaces of A and A' agree, and furthermore $p(1-q) = 1$ holds, these form a Riesz basis. □

Theorem 10.2 can be applied to the following example and its below mentioned generalisations.

Example 10.10 (Complex Robin boundary conditions)**.** Consider the interval $[0, a]$ and impose the boundary condition

$$\psi'(0) + (i\alpha - \beta)\psi(0) \quad \text{and} \quad \psi'(a) + (i\alpha + \beta)\psi(a) = 0, \quad \text{for } \alpha, \beta \in \mathbb{R},$$

cf [29, Sec. 6.3]. In matrix notation this becomes

$$A = \begin{bmatrix} i\alpha - \beta & 0 \\ 0 & -(i\alpha + \beta) \end{bmatrix} \quad \text{and} \quad B = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix},$$

hence one has also a parametrisation in terms of m-sectorial boundary conditions with $L = A$ and $P = 0$. Therefore, the operator $-\Delta(A, B)$ is defined by the form $\delta_{L,0}$ and Theorem 10.2 applies.

For $\beta = 0$ an explicit computation shows that the spectrum is real. Moreover, if $\alpha \neq n\pi/a$, $n \in \mathbb{N}$, all the eigenvalues have algebraic multiplicity one. We refer to [29] for more details.

In fact, it is well-known that the eigensystem $-\Delta(A,B)$ contains a Riesz basis (without brackets), [39], [13, Sec.XIX.3]. These boundary conditions were introduced in [29] as a toy quasi-self-adjoint model in $\mathcal{PT}$-symmetry and the closed formula for the metric operator has been found. An alternative method how to derive other closed formulae for the metric operators Θ was developed in [30] and further employed in [32], where one can additionally find an explicit formula for the self-adjoint operator to which $-\Delta(A,B)$ is similar. Notice that this self-adjoint operator is not a graph. The more general model with $\beta \neq 0$ is also studied in [31].

A generalisation of this example to metric graphs was proposed in [45]. Consider a compact star graph and the boundary conditions

$$A = \begin{bmatrix} A_+(\alpha) & 0 \\ 0 & A_- \end{bmatrix} \quad \text{and} \quad B = \begin{bmatrix} \mathbb{1} & 0 \\ 0 & B_- \end{bmatrix},$$

where $\{A_+(\alpha)\}_{lk} = i\alpha\delta_{lk}e^{2\pi i \frac{l}{\deg v}}$, $A_- = A_\nu$ and $B_- = B_\nu$ are the matrices given in (10.25) below defining the standard boundary conditions at the central vertex v with $\deg(v) = \nu$. Since the standard boundary conditions can be expressed equivalently by projectors P_ν and $P_\nu^\perp$, *cf* Subsection 10.6.5, one has that

$$L(\alpha) = \begin{bmatrix} A_+(\alpha) & 0 \\ 0 & 0 \end{bmatrix}, \quad \text{and} \quad P = \begin{bmatrix} 0 & 0 \\ 0 & P_\nu \end{bmatrix}.$$

Hence, Theorem 10.2 applies and there is a Riesz basis of projectors corresponding to invariant subspaces of $-\Delta(A,B)$.

Theorem 10.2 can be also applied to a compact graph with the combination of self-adjoint boundary conditions and complex δ-interactions, i.e. a modification of Example 10.4.

10.6 Quasi-self-adjointness for symmetric graphs

There are many works dealing with the question of similarity between non-self-adjoint and self-adjoint operators. In particular, there exists an abstract resolvent criterion for similarity to self-adjoint operators developed independently in [12], [37] and [41]. Based on this criteria, the question when operators with purely absolutely continuous spectrum are similar to self-adjoint ones was discussed in [15]. Another approach is through the framework of extension theory for symmetric operators [3, 21].

In this section we follow a completely different approach and succeed in reducing the question of quasi-self-adjointness for the unbounded operator $-\Delta(A,B)$ to a simple check of the similarity of $\mathfrak{S}(k,A,B)$ to a unitary matrix. The prize we pay is that the method applies to graphs with equal internal edge lengths only. More specifically, throughout this section, we always assume

$$a_i = a \qquad \text{for all} \qquad i \in \mathcal{I}. \tag{10.21}$$

10.6.1 From matrices to operators

For any $(|\mathcal{I}| \times |\mathcal{I}|)$-matrix $G(\mathcal{I}) = (G(\mathcal{I})_{ji})$ defining an operator in $\mathcal{K}_\mathcal{I}^-$ we introduce the map

$$\Phi_{G(\mathcal{I})}\colon \mathcal{H}_\mathcal{I} \to \mathcal{H}_\mathcal{I}, \quad \left(\Phi_{G(\mathcal{I})}\psi\right)(x_j) = \sum_{i=1}^n G(\mathcal{I})_{ji}\psi_i(x_j), \quad j \in \mathcal{I},$$

where $n = |\mathcal{I}|$. Accordingly, for a $(|\mathcal{E}| \times |\mathcal{E}|)$-matrix $G(\mathcal{E}) = (G(\mathcal{E})_{ji})$ defining an operator in $\mathcal{K}_\mathcal{E}$ we introduce

$$\Phi_{G(\mathcal{E})}\colon \mathcal{H}_\mathcal{E} \to \mathcal{H}_\mathcal{E}, \quad \left(\Phi_{G(\mathcal{E})}\psi\right)(x_j) = \sum_{i=1}^m G(\mathcal{E})_{ji}\psi_i(x_j), \quad j \in \mathcal{E},$$

where $m = |\mathcal{E}|$. These maps are well defined since the functions ψ_i are defined on the i-th edge, which is identified with a half-line or an interval $[0,a]$, respectively, and hence they can be interpreted as functions on another half-line or interval $[0,a]$ as well.

For any $\psi \in \mathcal{D}$ let us also define

$$\underline{\psi}_\mathcal{E} = \{\psi_e(0)\}_{e\in\mathcal{E}}, \qquad \underline{\psi}_{\mathcal{I},-} = \{\psi_i(0)\}_{i\in\mathcal{I}}, \qquad \underline{\psi}_{\mathcal{I},+} = \{\psi_i(a_i)\}_{i\in\mathcal{I}},$$
$$\underline{\psi}'_\mathcal{E} = \{\psi'_e(0)\}_{e\in\mathcal{E}}, \qquad \underline{\psi}'_{\mathcal{I},-} = \{\psi'_i(0)\}_{i\in\mathcal{I}}, \qquad \underline{\psi}'_{\mathcal{I},+} = \{-\psi'_i(a_i)\}_{i\in\mathcal{I}},$$

and

$$\underline{\psi}_\mathcal{I} = \underline{\psi}_{\mathcal{I},-} \oplus \underline{\psi}_{\mathcal{I},+}, \qquad \underline{\psi}'_\mathcal{I} = \underline{\psi}'_{\mathcal{I},-} \oplus \underline{\psi}'_{\mathcal{I},+}.$$

Finally, we set

$$\mathcal{D}_{\mathcal{E}} := \mathcal{D} \cap \mathcal{H}_{\mathcal{E}} \quad \text{and} \quad \mathcal{D}_{\mathcal{I}} := \mathcal{D} \cap \mathcal{H}_{\mathcal{I}}.$$

Here we collect basic properties of the maps $\Phi_{G(\mathcal{I})}$ and $\Phi_{G(\mathcal{E})}$.

Proposition 10.10. *The maps $\Phi_{G(\mathcal{E})}$ and $\Phi_{G(\mathcal{I})}$ are linear. For matrices G, H one has $\Phi_G \circ \Phi_H = \Phi_{G \circ H}$. In particular, if $G(\mathcal{I})$ or $G(\mathcal{E})$ is invertible, then $\Phi_{G(\mathcal{E})}$ respectively $\Phi_{G(\mathcal{I})}$ is invertible with*

$$\left(\Phi_{G(\mathcal{E})}\right)^{-1} = \Phi_{G(\mathcal{E})^{-1}} \quad \textit{and} \quad \left(\Phi_{G(\mathcal{I})}\right)^{-1} = \Phi_{G(\mathcal{I})^{-1}},$$

respectively. Furthermore $\Phi_{G(\mathcal{E})}$ maps $\mathcal{D}_{\mathcal{E}}$ to $\mathcal{D}_{\mathcal{E}}$ and $\Phi_{G(\mathcal{I})}$ maps $\mathcal{D}_{\mathcal{I}}$ to $\mathcal{D}_{\mathcal{I}}$. For $\psi \in \mathcal{D}_{\mathcal{E}}$ one has

$$\underline{\Phi_{G(\mathcal{E})}\psi}_{\mathcal{E}} = G(\mathcal{E})\, \underline{\psi}_{\mathcal{E}} \quad \textit{and} \quad \underline{\left(\Phi_{G(\mathcal{E})}\psi\right)'}_{\mathcal{E}} = G(\mathcal{E})\, \underline{\psi'}_{\mathcal{E}}.$$

For $\psi \in \mathcal{D}_{\mathcal{I}}$ one has

$$\underline{\Phi_{G(\mathcal{I})}\psi}_{\mathcal{I}} = \begin{bmatrix} G(\mathcal{I})\underline{\psi}_{\mathcal{I},-} \\ G(\mathcal{I})\underline{\psi}_{\mathcal{I},+} \end{bmatrix} \quad \textit{and} \quad \underline{\Phi_{G(\mathcal{I})}\psi'}_{\mathcal{I}} = \begin{bmatrix} G(\mathcal{I})\underline{\psi'}_{\mathcal{I},-} \\ G(\mathcal{I})\underline{\psi'}_{\mathcal{I},+} \end{bmatrix}.$$

10.6.2 The main result

Taking advantage of the transformation of the boundary values one obtains

Theorem 10.4. *Let $(\mathcal{G}, \underline{a})$ be a finite metric graph with equal internal edge lengths,* i.e. (10.21) *holds. Let A, B and A', B' be linear maps in $\mathcal{K}$ such that*

$$A' = G^{-1}AG \quad \textit{and} \quad B' = G^{-1}BG,$$

for an invertible operator G in $\mathcal{K}$ of the block diagonal form

$$G = \begin{bmatrix} G(\mathcal{E}) & 0 & 0 \\ 0 & G(\mathcal{I}) & 0 \\ 0 & 0 & G(\mathcal{I}) \end{bmatrix} \tag{10.22}$$

with $G(\mathcal{E})$ an invertible operator in $\mathcal{K}_{\mathcal{E}}$ and $G(\mathcal{I})$ an invertible operator in $\mathcal{K}_{\mathcal{I}}^-$. Then the Laplacians $-\Delta(A, B)$ and $-\Delta(A', B')$ are similar to each other, i.e.

$$\Phi_{G^{-1}}\Delta(A, B)\Phi_G = \Delta(A', B')$$

with similarity transform

$$\Phi_{G^{-1}} := \Phi_{G(\mathcal{E})^{-1}} \oplus \Phi_{G(\mathcal{I})^{-1}}. \tag{10.23}$$

Proof. Let $(\mathcal{G}, \underline{a})$ be a metric graph with equal internal edge lengths and

$$A' = G^{-1}AG \quad \text{and} \quad B' = G^{-1}BG,$$

where G is of the block-diagonal form given in the theorem. In order to prove that $\Delta(A', B') = \Phi_{G^{-1}}\Delta(A, B)\Phi_G$ one has to show

(a) $\Phi_{G^{-1}}$ maps $\mathsf{D}\Delta(A, B)$ to $\mathsf{D}\Delta(A', B')$;

(b) $\Phi_{G^{-1}}\Delta(A, B)\Phi_G\psi = \Delta(A', B')\psi$, for $\psi \in \mathsf{D}(A', B')$.

Note that Φ_G and $\Phi_{G^{-1}}$ commute with Δ, and therefore (b) holds.

It remains to show that $\Phi_{G^{-1}}(\mathsf{D}\Delta(A, B)) = \mathsf{D}(\Delta(A', B'))$. Since $\Phi_{G^{-1}}$ commutes with Δ, it follows also that $\Phi_{G^{-1}}\mathsf{R}\Delta(A, B) = \mathsf{R}\Delta(A', B')$. Consequently, by Lemma 10.10, $\Phi_{G^{-1}}$ maps $\mathcal{D}$ to $\mathcal{D}$. If $\psi \in \mathsf{D}(\Delta(A, B))$, then $\psi \in \mathcal{D}$ and (10.5) holds. Applying it to the function $\Phi_{G^{-1}}\psi$, we get

$$G^{-1}\left\{AGG^{-1}\underline{\psi} + BGG^{-1}\underline{\psi'}\right\} = 0,$$

therefore $\Phi_{G^{-1}}(\mathsf{D}(\Delta(A, B))) \subset \mathsf{D}(\Delta(A', B'))$. The other way round, one proves analogously $\Phi_G(\mathsf{D}(\Delta(A', B'))) \subset \mathsf{D}(\Delta(A, B))$. Since $\Phi_{G^{-1}}$ is a bijection this proves the claim. □

The main result of this section is now the following direct consequence of Theorem 10.4.

Corollary 10.4. *Let* $(\mathcal{G}, \underline{a})$ *be a finite metric graph with equal internal edge lengths,* i.e. (10.21) *holds.*

1. *Let* A, B *be linear maps in* $\mathcal{K}$ *such that*
$$\mathfrak{S}(k, A, B) = G^{-1} U G,$$
for an invertible operator G *in* $\mathcal{K}$ *of the block diagonal form* (10.22) *with* $G(\mathcal{E})$ *an invertible operator in* $\mathcal{K}_{\mathcal{E}}$ *and* $G(\mathcal{I})$ *an invertible operator in* $\mathcal{K}_{\mathcal{I}}^{-}$. *Then the Laplacians* $-\Delta(A, B)$ *and* $-\Delta(A_U, B_U)$ *with*
$$A_U := -\frac{1}{2}(U - \mathbb{1}) \quad \textit{and} \quad B_U := \frac{1}{2ik}(U + \mathbb{1}).$$
are similar to each other with the similarity transform given in (10.23). *In particular, if* U *is unitary then* $-\Delta(A, B)$ *is similar to a self-adjoint Laplacian.*

2. *Let* L, P *and* L', P' *define m-sectorial boundary conditions. Assume furthermore that there is an invertible operator* G *in* $\mathcal{K}$ *of the block diagonal form* (10.22) *with* $G(\mathcal{E})$ *an invertible operator in* $\mathcal{K}_{\mathcal{E}}$ *and* $G(\mathcal{I})$ *an invertible operator in* $\mathcal{K}_{\mathcal{I}}^{-}$ *such that*
$$P = G^{-1} P' G \quad \textit{and} \quad L = G^{-1} L' G.$$
Then $-\Delta(P+L, P^{\perp})$ *and* $-\Delta(P'+L', (P')^{\perp})$ *are similar to each other with the similarity transform given in* (10.23). *In particular, if* L' *is Hermitian then* $-\Delta(P + L, P^{\perp})$ *is similar to a self-adjoint Laplacian.*

Proof. Consider the boundary conditions
$$A_{\mathfrak{S}} := -\frac{1}{2}(\mathfrak{S} - \mathbb{1}) \quad \text{and} \quad B_{\mathfrak{S}} := \frac{1}{2ik}(\mathfrak{S} + \mathbb{1}),$$
and $k > 0$ such that $A_{\mathfrak{S}} + ikB_{\mathfrak{S}}$ is invertible, where $\mathfrak{S} := \mathfrak{S}(k, A, B)$. These are equivalent to the boundary conditions defined by A, B. By assumption there is an invertible operator G in $\mathcal{K}$ such that
$$A_{\mathfrak{S}} = G^{-1} A_U G \quad \text{and} \quad B_{\mathfrak{S}} = G^{-1} B_U G.$$
Applying Theorem 10.4 proves the claim. For m-sectorial boundary conditions the proof is analogous. □

Remark 10.7. Corollary 10.4 can be alternatively proven by using the resolvent formula given in Proposition 10.7 by proving the similarity of the resolvents where the similarity transforms are given by means of Φ_G.

10.6.3 Application to star graphs

Theorem 10.4 simplifies in the case of star graphs. Here a *non-compact star graph* is a graph with $\mathcal{I} = \emptyset$, and a *compact star graph with equal edge lengths* is a graph with $\mathcal{E} = \emptyset$ and $a_i = a$ for all $i \in \mathcal{I}$ such that $\partial_-(i) = \partial_-(i')$ for any $i, i' \in \mathcal{I}$ and $\partial_+(i) \neq \partial_+(i')$ whenever $i \neq i'$.

For a non-compact star graph consider the operator $-\Delta(A, B)$ where A, B are linear maps in $\mathcal{K}$. Two operators $-\Delta(A, B)$ and $-\Delta(A', B')$ are similar whenever there exists an invertible operator G in $\mathcal{K}_{\mathcal{E}}$ such that
$$A' = G^{-1} A G \quad \text{and} \quad B' = G^{-1} B G.$$
For the case of regular boundary conditions one has to check only if the matrices $\mathfrak{S}(k, A, B)$ and $\mathfrak{S}(k, A', B')$ are similar to each other.

In order to have an equally simple criterion for a compact star graph, one can consider $-\Delta(A, B)$ with boundary conditions of the form
$$A = \begin{bmatrix} A^{-} & 0 \\ 0 & A^{+} \end{bmatrix} \quad \text{and} \quad B = \begin{bmatrix} B^{-} & 0 \\ 0 & B^{+} \end{bmatrix}, \tag{10.24}$$
where A^{-}, B^{-} are arbitrary linear maps in $\mathcal{K}_{\mathcal{I}}^{-}$, and $A^{+} = a^{+}\mathbb{1}_{\mathcal{K}_{\mathcal{I}}^{+}}$ and $B^{+} = b^{+}\mathbb{1}_{\mathcal{K}_{\mathcal{I}}^{+}}$ with $a^{+}, b^{+} \in \mathbb{C}$.

Let A^{-}, B^{-} and A'^{-}, B'^{-} be linear maps in $\mathcal{K}^{-}$ such that
$$A'^{-} = G^{-1} A^{-} G \quad \text{and} \quad B'^{-} = G^{-1} B^{-} G,$$
for an invertible linear operator G in $\mathcal{K}^{-}$. Consider boundary conditions A', B' of the form (10.24) defined by A'^{-}, B'^{-} and $a^{+}, b^{+} \in \mathbb{C}$, and A, B also of the form (10.24) defined by A^{-}, B^{-} and the same numbers $a^{+}, b^{+} \in \mathbb{C}$. Then $-\Delta(A, B)$ and $-\Delta(A', B')$ are similar to each other with similarity transform $\Phi_{G^{-1}}$. Again, for the case of regular boundary conditions one has to check only if the matrices $\mathfrak{S}(k, A, B)$ and $\mathfrak{S}(k, A', B')$ are similar to each other. For taking into account only the boundary conditions at the central vertex it is crucial to impose identical boundary conditions at all endpoints.

Example 10.11 (Special case of Example 10.3)**.** Consider Example 10.3 for $|\mathcal{E}| = 3$, with $|\mathcal{E}_-| = 1$, $|\mathcal{E}_+| = 2$. Note that

$$\mathfrak{S}(k, A, B) = G \begin{bmatrix} 1 & 0 & 0 \\ 0 & -1 & 0 \\ 0 & 0 & -1 \end{bmatrix} G^{-1} \quad \text{with } G = \begin{bmatrix} 1 & -1 & 1 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \end{bmatrix}.$$

Hence, by Corollary 10.4, the operator $-\Delta(A, B)$ is unitarily equivalent to a self-adjoint Laplacian, namely to the direct sum of two Neumann Laplacians and one Dirichlet Laplacian on the half-line.

Example 10.12 (Star graph with both essential and discrete spectra)**.** Consider a star graph with only two external edges and the m-sectorial boundary conditions defined by

$$P = 0 \quad \text{and} \quad L = \begin{bmatrix} 0 & 2 \\ 1/2 & 0 \end{bmatrix},$$

that is $2\psi_2(0) + \psi_1'(0) = 0$ and $1/2\psi_1(0) + \psi_2'(0) = 0$. Since

$$L = \begin{bmatrix} 1/2 & 0 \\ 0 & 1/4 \end{bmatrix} L' \begin{bmatrix} 2 & 0 \\ 0 & 4 \end{bmatrix}, \quad \text{where } L' = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix},$$

one has by Corollary 10.4 that $-\Delta(L, \mathbb{1})$ is similar to the self-adjoint operator $-\Delta(L', \mathbb{1})$. Hence, the continuous spectrum of $-\Delta(L, \mathbb{1})$ is $[0, \infty)$ and the point spectrum contains only the isolated simple eigenvalue -1.

10.6.4 Application to Example 10.5

During our work we had in mind, as a guiding example, the class of point interactions defined at point zero on the intervals $(-L, L)$, $L \in (0, +\infty]$ by

$$\begin{bmatrix} \psi(0+) \\ \psi'(0+) \end{bmatrix} = \begin{bmatrix} e^{i\tau} & 0 \\ 0 & e^{-i\tau} \end{bmatrix} \begin{bmatrix} \psi(0-) \\ \psi'(0-) \end{bmatrix} \quad \text{for } \tau \in [0, \pi/2],$$

which is also discussed in Example 10.5 above. Actually, this has been the starting point of our study, and now we are in the position to apply our results to reproduce some of the results known for it.

Regular case

Let $\tau \in [0, \pi/2)$. For the Cayley transform

$$\mathfrak{S}(A_\tau, B_\tau, k) = -(A_\tau + ikB_\tau)^{-1}(A_\tau - ikB_\tau),$$

an explicit computation yields the diagonalisation

$$\frac{1}{\cos(\tau)} \begin{bmatrix} i\sin(\tau) & 1 \\ 1 & -i\sin(\tau) \end{bmatrix} = \frac{-1}{2\cos(\tau)} \begin{bmatrix} 1 & 1 \\ e^{-i\tau} & -e^{i\tau} \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} -e^{i\tau} & -1 \\ -e^{-i\tau} & 1 \end{bmatrix}.$$

Hence, one has using $\operatorname{diag}\{1, -1\} = Q\mathfrak{S}(A_0, B_0, k)Q$ the similarity

$$\mathfrak{S}(A_\tau, B_\tau, k) = G_\tau^{-1} Q\mathfrak{S}(A_0, B_0, k)QG_\tau,$$

where

$$Q = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \quad \text{and} \quad G_\tau = \frac{i}{\sqrt{2\cos(\tau)}} \begin{bmatrix} -e^{i\tau} & -1 \\ -e^{-i\tau} & 1 \end{bmatrix}.$$

From Corollary 10.4 it follows that the operator $-\Delta(A_\tau, B_\tau)$ is similar to the self-adjoint Laplacian $-\Delta(A_0, B_0)$, and the similarity transform is given by Φ_{QG_τ}:

$$\Delta(A_0, B_0) = \Phi_{(QG_\tau)^{-1}} \Delta(A_\tau, B_\tau) \Phi_{QG_\tau}.$$

In fact, $-\Delta(A_0, B_0)$ is the standard Laplacian on the real line.

One can now compute a metric operator, *i.e.* the operator Θ_τ such that

$$\Delta(A_\tau, B_\tau)^* = \Theta_\tau \Delta(A_\tau, B_\tau) \Theta_\tau^{-1}.$$

Since Q is unitary, a metric is given by the formula

$$\Theta_\tau = \Phi_{(G_\tau^* G_\tau)^{-1}}, \quad \text{where} \quad (G_\tau^* G_\tau)^{-1} = \frac{1}{\cos(\tau)} \begin{bmatrix} 1 & i\sin(\tau) \\ -i\sin(\tau) & 1 \end{bmatrix}.$$

We also have $\Theta_\tau^{-1} = \Phi_{G_\tau^* G_\tau}$, where

$$G_\tau^* G_\tau = \frac{1}{\cos(\tau)} \begin{bmatrix} 1 & -i\sin(\tau) \\ i\sin(\tau) & 1 \end{bmatrix}.$$

One can rewrite this as

$$\Theta_\tau = \frac{1}{\cos(\tau)} \left[\mathbb{1} - i\sin(\tau) M_{\mathrm{sgn}} \mathcal{P}\right] \quad \text{and} \quad \Theta_\tau^{-1} = \frac{1}{\cos(\tau)} \left[\mathbb{1} + i\sin(\tau) M_{\mathrm{sgn}} \mathcal{P}\right].$$

Here the operator $\mathcal{P}$ interchanges the edges (therefore it corresponds in fact to the parity operator in a quantum-mechanical interpretation of the model) and M_{sgn} denotes the multiplication by $+1$ on the first edge and by -1 on the second edge (therefore, identifying the graph with the real line, M_{sgn} corresponds to the multiplication by sgn). This is, up to a constant factor, the metric operator given in [44, Chap. 2.5].

Considering the same boundary conditions at the central vertex on the compact star graph with two edges one obtains that the operators is similar to a self-adjoint Laplacian for any self-adjoint boundary condition imposed at both endpoints simultaneously, in particular for Dirichlet boundary conditions as considered in [44, Chap. 2.5]. In all cases a similarity transform is given by Φ_{QG_τ} and a metric operator is given by $\Phi_{(G_\tau^* G_\tau)^{-1}}$.

Irregular case

Let $\tau = \pi/2$. One has

$$\begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} = \frac{1}{2} A_{\pi/2} \begin{bmatrix} 1 & 1 \\ -i & i \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} = \frac{1}{2} B_{\pi/2} \begin{bmatrix} 1 & 1 \\ -i & i \end{bmatrix}.$$

Hence, by Theorem 10.4, the operator $-\Delta(A_{\pi/2}, B_{\pi/2})$ on the star graph with only two external edges is unitarily equivalent to $-\Delta(A', B')$ with

$$A' = \begin{bmatrix} 0 & 1 \\ 0 & 0 \end{bmatrix} \quad \text{and} \quad B' = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}.$$

These boundary conditions are $\psi_2(0) = \psi_2'(0) = 0$, that is $-\Delta(A', B')$ is the direct sum of the minimal operator $-\Delta^0$ on one edge and the maximal operator $-\Delta$ on the other edge. Recall that $\sigma(-\Delta(A_{\pi/2}, B_{\pi/2})) = \mathbb{C}$.

Irregular compact case

Consider a compact star graph and let more generally A^-, B^- define arbitrary irregular boundary conditions at the central vertex, and let a^+, b^+ with $\mathrm{Rank}(a^+,\, b^+) = 1$ define boundary conditions at the end points, such that one obtains boundary conditions of the form (10.24). Hence there is a $\underline{\psi} \in \mathsf{N}A^- \cap \mathsf{N}B^- \neq \{0\}$ with $\|\underline{\psi}\| = 1$ and there is a unitary map in $\mathcal{K}$ mapping $\underline{\psi}$ to a unit vector e_i, $i \in \mathcal{I}$. The boundary conditions

$$A'^- = A^- U \quad \text{and} \quad B'^- = B^- U$$

define a unitarily equivalent operator, but the edge i is decoupled from the rest of the graph and the operator on this edge has domain

$$\{\psi \in \mathcal{D}_j \mid a^+ \psi(a) - b^+ \psi'(a) = 0\}$$

which defines by Proposition 10.5 operator with entire $\mathbb{C}$ in the spectrum. This shows that also the operator defined on a compact star graph with only two internal edges of equal length where the boundary conditions at the central vertex are given by $A_{\pi/2}, B_{\pi/2}$ and at the endpoint arbitrary regular boundary conditions are imposed has empty resolvent set. This reproduces some of the result from [44, Chap. 2.5].

Relation to Example 10.1

Consider the boundary conditions defined by

$$A = \begin{bmatrix} 1 & -1 \\ 0 & 0 \end{bmatrix} \quad \text{and} \quad B = \begin{bmatrix} 0 & 0 \\ 1 & -1 \end{bmatrix}.$$

Then one obtains

$$\frac{1}{\sqrt{2}} AU = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}, \quad \tfrac{1}{\sqrt{2}} BU = \begin{bmatrix} 0 & 0 \\ 1 & 0 \end{bmatrix}, \quad \text{where } U = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix},$$

and U maps $\mathsf{N}A \cap \mathsf{N}B$ to $\operatorname{span}\{e_2\}$. These boundary conditions define on one edge the minimal operator $-\Delta^0$ and on the other edge the maximal operator $-\Delta$. For a compact star graph with these boundary conditions at the central vertex the same holds.

Note that for $A_{\pi/2}, B_{\pi/2}$ one has

$$\begin{bmatrix} 1 & -1 \\ 0 & 0 \end{bmatrix} = A_{\pi/2} \begin{bmatrix} 1 & 0 \\ 0 & -i \end{bmatrix} \quad \text{and} \quad \begin{bmatrix} 0 & 0 \\ 1 & -1 \end{bmatrix} = B_{\pi/2} \begin{bmatrix} 1 & 0 \\ 0 & -i \end{bmatrix},$$

hence the operator defined by $A_{\pi/2}, B_{\pi/2}$ at the central vertex of a star graph with two edges of equal, possibly infinite, length is unitarily equivalent to the operator $-\operatorname{sgn}(x)\frac{d}{dx}\operatorname{sgn}(x)\frac{d}{dx}$, if in addition at the endpoint the same boundary conditions are imposed.

10.6.5 Applications to self-adjoint Laplacians

Theorem 10.4 and its Corollary 10.4 can also be interestingly applied to self-adjoint Laplacians, in order to simplify the computation of the spectrum. Consider a compact star graph (see Figure 10.1(a) for an example with three edges) with standard (or Kirchhoff) boundary condition at the central vertex v, where $\deg(v) = \nu$, *i.e.*

$$A_\nu = \begin{bmatrix} 1 & -1 & 0 & \cdots & 0 & 0 \\ 0 & 1 & -1 & \cdots & 0 & 0 \\ 0 & 0 & 1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 1 & -1 \\ 0 & 0 & 0 & \cdots & 0 & 0 \end{bmatrix}, \qquad B_\nu = \begin{bmatrix} 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 0 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & 0 & 0 \\ 1 & 1 & 1 & \cdots & 1 & 1 \end{bmatrix}. \tag{10.25}$$

It is known that

$$[\mathfrak{S}(k, A_\nu, B_\nu)]_{ij} = \frac{2}{\deg(v)} - \delta_{ij},$$

see, *e.g.*, [24, Ex. 2.4], and furthermore, it admits the representation

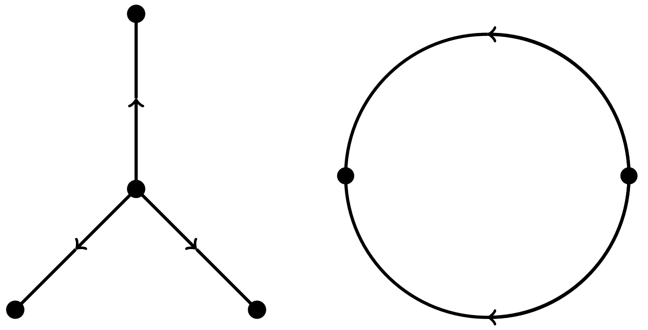
$$\mathfrak{S}(k, A_\nu, B_\nu) = P_\nu^\perp - P_\nu,$$

where P_ν is the orthogonal projector onto $\mathsf{N}B_\nu$ and its complementary projector $P_\nu^\perp = \mathbb{1} - P_\nu$ is the orthogonal projector onto the space spanned by the vector $\{w_\nu\}_j = 1$, $j = 1, \ldots, \deg(v)$. Hence $\mathfrak{S}(k, A_\nu, B_\nu)$ has the eigenvalues -1 of multiplicity $\deg(v) - 1$ and $+1$ of simple multiplicity. At the ends of the leads one imposes for example Dirichlet boundary conditions. Then by applying Theorem 10.4 one obtains that this operator is iso-spectral to a direct sum of operators on intervals. Namely, $\deg(v) - 1$ Dirichlet Laplacians on intervals $[0, a]$ and one Laplacian on $[0, a]$ with Dirichlet boundary condition at a and Neumann boundary condition at 0. This provides a complete picture of the spectrum. The spectrum is purely discrete and the solutions k_n, $n \in \mathbb{N}$, of $\sin(ka) = 0$ yield eigenvalues k_n^2 of multiplicity $\deg(v) - 1$ and the solutions k_m, $m \in \mathbb{N}$, of $\cos(ka) = 0$ yield eigenvalues k_m^2 of multiplicity one.

Consider as a further example a compact graph consisting of two vertices $V = \{v_1, v_2\}$ connected by n edges $\mathcal{I} = \{i_1, \ldots, i_n\}$ of the same length $a > 0$ (see Figure 10.1(b) for an example with two edges which is in fact a loop). Each of the two vertices is a vertex of degree $\nu = n$, and now one imposes at each vertex the standard boundary conditions (10.25).

For this graph the boundary conditions have the following block structure

$$A = \begin{bmatrix} A_{++} & 0 \\ 0 & A_{--} \end{bmatrix} \quad \text{and} \quad B = \begin{bmatrix} B_{++} & 0 \\ 0 & B_{--} \end{bmatrix}$$



(a) A compact star graph (b) Loop as a graph with two vertices

Figure 10.1: Graphs considered in Subsection 10.6.5

with respect to the decomposition $\mathcal{K}_{\mathcal{I}} = \mathcal{K}_{\mathcal{I}}^{+} \oplus \mathcal{K}_{\mathcal{I}}^{-}$. Furthermore $A_{++} = A_{--}$ and $B_{++} = B_{--}$, where

$$A_{++} = A_{\nu} \quad \text{and} \quad B_{++} = B_{\nu},$$

where A_{ν} and B_{ν} are the matrices from (10.25). Applying as in the previous example the diagonalisation of $\mathfrak{S}(k, A_{\nu}, B_{\nu})$ one arrives at the conclusion that the Laplacian $-\Delta(A, B)$ with standard boundary conditions on the this graph with two vertices is unitarily equivalent to the direct sum of $(n-1)$ copies of the Dirichlet Laplacian on the interval of length a and one copy of the Neumann Laplacian on such an interval. This gives immediately the spectrum of the operator which is is purely discrete, and given by the eigenvalue zero of multiplicity one and by the eigenvalues k_m^2 of multiplicity n, where k_m, $m \in \mathbb{N}$, solves the equation $\sin(ka) = 0$.

More generally, one can consider such a compact graph where at both vertices one imposes the same boundary conditions. For instance, consider such a compact graph with two edges $\mathcal{I} = \{i_1, i_2\}$ of equal length $a > 0$ and two vertices $V = \{v_1, v_2\}$ with $\partial^{+}(i_1) = \partial^{+}(i_2)$ and $\partial^{-}(i_1) = \partial^{-}(i_2)$, that is a loop with two vertices. One imposes at each vertex boundary conditions A_{τ}, B_{τ} given in Example 10.5, both with the same $\tau \in [0, \pi/2)$. Applying Corollary 10.4 delivers that the corresponding operator is similar to the Laplacian on the circle with arc length $2a$.

10.7 Appendix

This appendix is devoted to the proof of Proposition 10.7.

Definition 10.3 ([27, Def. 3.9])**.** The operator $\mathfrak{K}$ on the Hilbert space $\mathcal{H}$ is called *integral operator* if for all $j, j' \in \mathcal{E} \cup \mathcal{I}$ there are measurable functions $\mathfrak{K}_{j,j'}(\cdot,\cdot)\colon I_j \times I_{j'} \to \mathbb{C}$ with the following properties

1. $\mathfrak{K}_{j,j'}(x_j, \cdot)\varphi_{j'} \in L^1(I_{j'})$ for almost all $x_j \in I_j$,
2. $\psi = \mathfrak{K}\varphi$ with
$$\psi_j(x_j) = \sum_{j' \in \mathcal{E} \cup \mathcal{I}} \int_{I_{j'}} \mathfrak{K}_{j,j'}(x_j, y_{j'})\varphi_{j'}(y_{j'})dy_{j'}.$$

The $(\mathcal{I} \cup \mathcal{E}) \times (\mathcal{I} \cup \mathcal{E})$ matrix-valued function $(x, y) \mapsto \mathfrak{K}(x, y)$ with

$$[\mathfrak{K}(x, y)]_{j,j'} = \mathfrak{K}_{j,j'}(x_j, y_{j'})$$

is called the *integral kernel* of the operator $\mathfrak{K}$.

In order to prove Proposition 10.7, we adapt the proof of [24, Lem. 4.2], where the resolvents of self–adjoint Laplace operators are considered, to the situation of more general regular boundary conditions.

By assumption the operator $\mathfrak{S}(k, A, B)$ is defined and $\mathbb{1} - \mathfrak{S}(k, A, B)T(k; \underline{a})$ is invertible for k with $\Im k > 0$. Hence the kernel $r_{\mathcal{M}}(x, y; k)$ defined in Proposition 10.7 is well-defined, and with $\Im k > 0$ it defines a bounded operator $R_{\mathcal{M}}(k)$ in $\mathcal{H}$ by

$$R_{\mathcal{M}}(k)\varphi = \int_{\mathcal{G}} r_{\mathcal{M}}(\cdot, y; k)\varphi \quad \text{for } \varphi \in \mathcal{H}.$$

In order to prove that $R_{\mathcal{M}}(k)$ defines the resolvent operator, it suffices to check

(i) $R_{\mathcal{M}}(k)\varphi \in \mathsf{D}(\Delta(A,B))$, for all $\varphi \in \mathcal{H}$,

(ii) $(-\Delta(A,B) - k^2)R_{\mathcal{M}}(k)\varphi = \varphi$ for all $\varphi \in \mathcal{H}$ and

(iii) the symmetry relation $r_{\mathcal{M}}(y,x;k)^* = r_{\mathcal{M}^*}(x,y,-\overline{k})$.

The first two assertions prove that $(-\Delta(A,B)-k^2)R_{\mathcal{M}}(k) = \mathbb{1}_{\mathcal{H}}$ that is, $R_{\mathcal{M}}(k)$ is the right inverse. By (iii) one proves that also $(-\Delta(A,B)^* - \overline{k}^2)R(k)^*_{\mathcal{M}} = \mathbb{1}_{\mathcal{H}}$, and taking the adjoints one obtains $R_{\mathcal{M}}(k)(-\Delta(A,B) - k^2) \subset \mathbb{1}_{\mathcal{H}}$. This proves that $R_{\mathcal{M}}(k)$ is also the left inverse.

Using [24, Lem. 4.2] and (10.16), one can also rewrite $r_{\mathcal{M}}(x,y;k)$ as

$$
\begin{aligned}
r_{\mathcal{M}}(x,y;k) &= r^0(x,y;k) + r^1_{\mathcal{M}}(x,y;k),\\
r^1_{\mathcal{M}}(x,y;k) &= -\frac{i}{2k}\Phi(x,k)Z(k;A,B,\underline{a})^{-1}(A-ikB)R_+(k;\underline{a})^{-1}\Phi(y,k)^T.
\end{aligned}
$$

One can still prove (i) and (ii) whenever $Z(k;A,B,\underline{a})$ is invertible proving that $R(k)$ defines the right inverse, but one cannot use the same proof for showing that the symmetry relation (iii) holds.

Proof of (i). With $\psi = R_{\mathcal{M}}(k)\varphi$, for $\varphi \in \mathcal{H}$ one has clearly $\psi \in \mathcal{D}$. Furthermore, set for brevity

$$G(k) := -Z(k;A,B,\underline{a})^{-1}(A-ikB)R_+(k,\underline{a})^{-1}.$$

Assume that $\varphi_j \in \mathcal{H}_j$ vanishes in a small neighbourhood of $x_j = 0$ and, in addition, in a small neighbourhood of $x_j = a_j$ if $j \in \mathcal{I}$. Then

$$\int_{I_j} e^{ik|x_j-y_j|}\varphi_j(y_j)dy_j = \int_{I_j} e^{-ik(x_j-y_j)}\varphi_j(y_j)dy_j$$

holds for sufficiently small $x_j \in I_j$, and for $x_j \in I_j$ sufficiently close to a_j one has

$$\int_{I_j} e^{ik|x_j-y_j|}\varphi_j(y_j)dy_j = \int_{I_j} e^{ik(x_j-y_j)}\varphi_j(y_j)dy_j.$$

Therefore one obtains for the traces

$$
\begin{aligned}
\underline{\psi} &= \frac{i}{2k}R_+(k;\underline{a})^{-1}\int_{\mathcal{G}}\Phi(y,k)^T\varphi(y)dy + \frac{i}{2k}X(k;\underline{a})G(k)\int_{\mathcal{G}}\Phi(y,k)^T\varphi(y)dy,\\
\underline{\psi}' &= \frac{1}{2}R_+(k;\underline{a})^{-1}\int_{\mathcal{G}}\Phi(y,k)^T\varphi(y)dy - \frac{1}{2}Y(k;\underline{a})G(k)\int_{\mathcal{G}}\Phi(y,k)^T\varphi(y)dy.
\end{aligned}
$$

Hence,

$$
\begin{aligned}
A\underline{\psi} + B\underline{\psi}' &= \frac{i}{2k}\left\{(A-ikB)R_+(k;\underline{a})^{-1} + Z(k;A,B,\underline{a})G(k)\right\}\int_{\mathcal{G}}\Phi(y,k)^T\varphi(y)dy\\
&= 0.
\end{aligned}
$$

Thus $R_{\mathcal{M}}(k)$ maps a dense subset of $\mathcal{H}$ to $\mathsf{D}(\Delta(A,B))$. By continuous continuation the claim follows for all $\varphi \in \mathcal{H}$ which proves (i). □

Proof of (ii). Assume that $\varphi_j \in C_0^\infty(I_j)$ for every $j \in \mathcal{I}\cup\mathcal{E}$. Since $\frac{i}{2k}e^{ik|x-y|}$ defines the Green's function on the real line it follows that

$$-\frac{i}{2k}\left(\frac{d^2}{dx_j^2} + k^2\right)\int_{I_j} e^{ik|x_j-y_j|}\varphi_j(y_j)dy_j = \varphi_j(x_j), \quad j \in \mathcal{I}\cup\mathcal{E}.$$

Note that the remainder vanishes, and therefore one has proven the identity

$$\left(-\Delta(A,B) - k^2\right)R_{\mathcal{M}}(k)\varphi = \varphi$$

for a dense subset of $\mathcal{H}$ and by continuous continuation the claim follows. □

Proof of (iii). The relation $r^0(y,x;k)^* = r^0(x,y,-\overline{k})$ can be verified directly. For the remainder one obtains

$$
\begin{aligned}
r^1_{\mathcal{M}}(y,x,k)^* = &\frac{i}{2(-\overline{k})}\Phi(x,-\overline{k})R_+(-\overline{k};\underline{a})^{-1}\mathfrak{S}(k,A,B)^*\\
&\times\left[\mathbb{1} - T(-\overline{k};\underline{a})\mathfrak{S}(k,A,B)^*\right]^{-1}R_+(-\overline{k};\underline{a})^{-1}\Phi(y,-\overline{k})^T,
\end{aligned}
$$

Note that

$$\mathfrak{S}(k,A,B)^* \left[\mathbb{1} - T(-\overline{k};\underline{a})\mathfrak{S}(k,A,B)^*\right]^{-1} = \left[\mathbb{1} - \mathfrak{S}(k,A,B)^* T(-\overline{k};\underline{a})\right]^{-1} \mathfrak{S}(k,A,B)^*$$

and $\mathfrak{S}(k,A,B)^* = \mathfrak{S}(-\overline{k},A',B')$, where

$$A' := -\frac{1}{2}\left(\mathfrak{S}(k,A,B)^* - \mathbb{1}\right) \quad \text{and} \quad B' := \frac{1}{-2i\overline{k}}\left(\mathfrak{S}(k,A,B)^* + \mathbb{1}\right).$$

From Proposition 10.3 it follows that $r^1_{\mathcal{M}}(y,x;k)^* = r^1_{\mathcal{M}^*}(x,y;-\overline{k})$, and therefore $R_{\mathcal{M}}(k)^* = R_{\mathcal{M}^*}(-\overline{k})$. □

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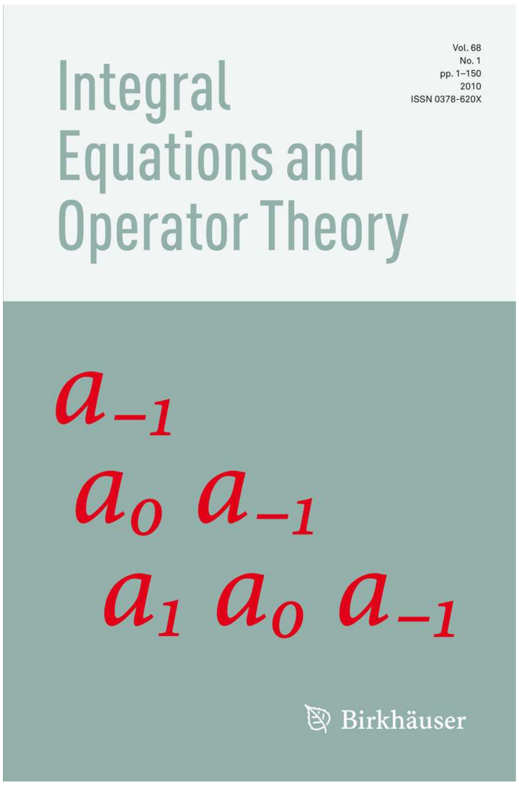
Part II

Waveguides

Chapter 11

$\mathcal{PT}$-symmetric waveguides



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Joint work with: Denis Borisov

$\mathcal{PT}$-symmetric waveguides

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Abstract. We introduce a planar waveguide of constant width with non-Hermitian $\mathcal{PT}$-symmetric Robin boundary conditions. We study the spectrum of this system in the regime when the boundary coupling function is a compactly supported perturbation of a homogeneous coupling. We prove that the essential spectrum is positive and independent of such perturbation, and that the residual spectrum is empty. Assuming that the perturbation is small in the supremum norm, we show that it gives rise to real weakly-coupled eigenvalues converging to the threshold of the essential spectrum. We derive sufficient conditions for these eigenvalues to exist or to be absent. Moreover, we construct the leading terms of the asymptotic expansions of these eigenvalues and the associated eigenfunctions.

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Keywords: non-self-adjointness, J-self-adjointness, $\mathcal{PT}$-symmetry, waveguides, Robin boundary conditions, Robin Laplacian, eigenvalue and eigenfunction asymptotics, essential spectrum, reality of the spectrum.

11.1 Introduction

There are two kinds of motivations for the present work. The first one is due to the growing interest in spectral theory of non-self-adjoint operators. It is traditionally relevant to the study of dissipative processes, resonances if one uses the mathematical tool of complex scaling, and many others. The most recent and conceptually new application is based on the potential quantum-mechanical interpretation of non-Hermitian Hamiltonians which have real spectra and are invariant under a simultaneous $\mathcal{P}$-parity and $\mathcal{T}$-time reversal. For more information on the subject, we refer to the pioneering work [3] and especially to the recent review [2] with many references.

The other motivation is due to the interesting phenomena of the existence of bound states in quantum-waveguide systems intensively studied for almost two decades. Here we refer to the pioneering work [12] and to the reviews [10, 21]. In these models the Hamiltonian is self-adjoint and the bound states – often without classical interpretations – correspond to an electron trapped inside the waveguide.

In this paper we unify these two fields of mathematical physics by considering a quantum waveguide modelled by a non-Hermitian $\mathcal{PT}$-symmetric Hamiltonian. Our main interest is to develop a spectral theory for the Hamiltonian and demonstrate the existence of eigenvalues outside the essential spectrum. For non-self-adjoint operators the location of the various essential spectra is often as much as one can realistically hope for in the absence of the powerful tools available when the operators are self-adjoint, notably the spectral theorem and minimax principle. In the present paper we overcome this difficulty by using perturbation methods to study the point spectrum in the weak-coupling regime. In certain situations we are also able to prove that the total spectrum is real.

Let us now briefly recall the notion of $\mathcal{PT}$-symmetry. If the underlying Hilbert space of a Hamiltonian H is the usual realization of square integrable functions $L^2(\mathbb{R}^n)$, the $\mathcal{PT}$-symmetry invariance can be stated in terms of the commutator relation

$$(\mathcal{PT})H = H(\mathcal{PT})\,, \tag{11.1}$$

where the parity and time reversal operators are defined by $(\mathcal{P}\psi)(x) := \psi(-x)$ and $\mathcal{T}\psi := \overline{\psi}$, respectively. In most of the $\mathcal{PT}$-symmetric examples H is the Schrödinger operator $-\Delta + V$ with a potential V satisfying (11.1), so that $H^* = \mathcal{T}H\mathcal{T}$ where H^* denotes the adjoint of H. This property is known as the $\mathcal{T}$-self-adjointness of H in the mathematical literature [11], and it is not limited to $\mathcal{PT}$-symmetric Schrödinger operators. More generally, given any linear operator H in an abstract Hilbert space $\mathcal{H}$, we understand the $\mathcal{PT}$-symmetry property as a special case of the J-self-adjointness of H:

$$H^* = JHJ\,, \tag{11.2}$$

where J is a conjugation operator, *i.e.*,

$$\forall \phi, \psi \in \mathcal{H}\,, \qquad (J\phi, J\psi)_{\mathcal{H}} = (\psi, \phi)_{\mathcal{H}}\,, \quad J^2\psi = \psi\,.$$

This setting seems to be adequate for a rigorous formulation of $\mathcal{PT}$-symmetric problems, and alternative to that based on Krein spaces [22, 24].

The nice feature of the property (11.2) is that H "is not too far" from the class of self-adjoint operators. In particular, the eigenvalues are found to be real for many $\mathcal{PT}$-symmetric Hamiltonians [28, 9, 22, 8, 26, 7, 20]. However, the situation is much less studied in the case when the resolvent of H is not compact.

The spectral analysis of non-self-adjoint operators is more difficult than in the self-adjoint case, partly because the residual spectrum is in general not empty for the former. One of the goals of the present paper is to point out that the existence of this part of spectrum is always ruled out by (11.2):

Fact. *Let H be a densely defined closed linear operator in a Hilbert space satisfying* (11.2)*. Then the residual spectrum of H is empty.*

The proof follows easily by noticing that the kernels of $H-\lambda$ and $H^*-\overline{\lambda}$ have the same dimension [11, Lem. III.5.4] and by the the general fact that the orthogonal complement of the range of a densely defined closed operator in a Hilbert space is equal to the kernel of its adjoint. The above result is probably not well known in the $\mathcal{PT}$-symmetry community.

We continue with an informal presentation of our model and main spectral results obtained in this paper. The rigorous and more detailed statements are postponed until the next section because they require a number of technical definitions.

The Hamiltonian we consider in this paper acts as the Laplacian in the Hilbert space of square integrable functions over a straight planar strip and the non-Hermiticity enters through $\mathcal{PT}$-symmetric boundary conditions only. The boundary conditions are of Robin type but with imaginary coupling. The $\mathcal{PT}$-symmetric invariance then implies that we actually deal with an electromagnetic waveguide with radiation/dissipative boundary conditions. In fact, the one-dimensional spectral problem in the waveguide cross-section has been studied recently in [20] (see also [19]) and our model can be viewed as a two-dimensional extension of the former.

Schrödinger-type operators with similar non-Hermitian boundary conditions were studied previously by Kaiser, Neidhardt and Rehberg [17, 16, 15]. In their papers, motivated by the needs of semiconductor physics, the configuration space is a bounded domain and the boundary coupling function is such that the Hamiltonian is a dissipative operator. The latter excludes the $\mathcal{PT}$-symmetric models of [20] and the present paper.

The $\mathcal{T}$-self-adjointness property (11.2) of our Hamiltonian is proved in Section 11.3. If the boundary coupling function is constant, the spectral problem can be solved by separation of variables and we find that the spectrum is purely essential, given by a positive semibounded interval (*cf* Section 11.4). In Section 11.5 we prove that the essential spectrum is stable under compactly supported perturbations of the coupling function. Consequently, the essential spectrum is always real in our setting, however, it exhibits important differences as regards similar self-adjoint problems. Namely, it becomes as a set independent of the value of the coupling function at infinity when the latter overpasses certain critical value.

In Section 11.6 we study the point spectrum. We focus on the existence of eigenvalues emerging from the threshold of the essential spectrum in the limit when the compactly supported perturbation of the coupling function tends to zero in the supremum norm. It turns out that the weakly-coupled eigenvalues may or may not exist, depending on mean values of the local perturbation. In the case when the point spectrum exists, we derive asymptotic expansions of the eigenvalues and the associated eigenfunctions.

Because of the singular nature of the $\mathcal{PT}$-symmetric interaction, our example is probably the simplest non-trivial, multidimensional $\mathcal{PT}$-symmetric model whatsoever for which both the point and essential spectra exist. We hope that the present work will stimulate more research effort in the direction of spectral and scattering properties of the present and other non-Hermitian $\mathcal{PT}$-symmetric operators.

11.2 Main results

Given a positive number d, we write $I := (0,d)$ and consider an infinite straight strip $\Omega := \mathbb{R}\times I$. We split the variables consistently by writing $x=(x_1,x_2)$ with $x_1\in\mathbb{R}$ and $x_2\in I$. Let α be a bounded real-valued function on $\mathbb{R}$; occasionally we shall denote by the same symbol the function $x\mapsto\alpha(x_1)$ on Ω. The object of our interest is the operator in the Hilbert space $L^2(\Omega)$ which acts as the Laplacian and satisfies the following $\mathcal{PT}$-symmetric boundary conditions:

$$\partial_2\Psi+\mathrm{i}\,\alpha\,\Psi\,=\,0 \qquad \text{on} \quad \partial\Omega\,. \tag{11.3}$$

More precisely, we introduce

$$H_\alpha\Psi:=-\Delta\Psi\,,\qquad \Psi\in\mathsf{D}(H_\alpha):=\left\{\Psi\in W_2^2(\Omega)\,|\,\Psi\text{ satisfies (11.3)}\right\}\,, \tag{11.4}$$

where the action of H_α should be understood in the distributional sense and (11.3) should be understood in the sense of traces [1]. In Section 11.3 we show that H_α is well defined in the sense that it is an m-sectorial operator and that its adjoint is easy to identify:

Theorem 11.1. *Let $\alpha \in W^1_\infty(\mathbb{R})$. Then H_α is an m-sectorial operator in $L^2(\Omega)$ satisfying*

$$H_\alpha^* = H_{-\alpha}\,. \tag{11.5}$$

Of course, H_α is not self-adjoint unless α vanishes identically (in this case H_0 is the Neumann Laplacian in $L^2(\Omega)$). However, H_α is $\mathcal{T}$-self-adjoint, *i.e.*, it satisfies (11.2) with J being the complex conjugation $\mathcal{T} : \Psi \mapsto \overline{\Psi}$. Indeed, H_α satisfies the relation (11.5) and it is easy to see that

$$H_{-\alpha} = \mathcal{T} H_\alpha \mathcal{T}\,. \tag{11.6}$$

This reflects the $\mathcal{PT}$-symmetry (11.1) of our problem, with $\mathcal{P}$ being defined by $(\mathcal{P}\Psi)(x) := \Psi(x_1, d - x_2)$.

An important property of an operator H in a Hilbert space $\mathcal{H}$ being m-sectorial is that it is closed. Then, in particular, the spectrum $\sigma(H)$ is well defined as the set of complex points z such that $H - z$ is not bijective as the operator from $\mathsf{D}(H)$ to $\mathcal{H}$. Furthermore, its spectrum is contained in a sector of complex numbers z such that $|\arg(z - \gamma)| \leqslant \theta$ with some $\gamma \in \mathbb{R}$ and $\theta \in [0, \pi/2)$. In our case, however, we are able to establish a stronger result

$$\sigma(H_\alpha) \;\subseteq\; \Xi_\alpha := \left\{ z \in \mathbb{C} \,:\, \operatorname{Re} z \geqslant 0\,,\ |\operatorname{Im} z| \leqslant 2\,\|\alpha\|_{L_\infty(\mathbb{R})} \sqrt{\operatorname{Re} z} \right\}. \tag{11.7}$$

This follows directly from Lemma 11.1 on which the proof of Theorem 11.1 is based (*cf* the end of Section 11.3 for more details). Consequently, the resolvent set $\rho(H_\alpha) := \mathbb{C} \setminus \sigma(H_\alpha)$ contains the complement of Ξ_α and we have the bound

$$\|(H_\alpha - z)^{-1}\| \;\leq\; 1/\operatorname{dist}(z, \partial\Xi_\alpha) \qquad \text{for all} \quad z \in \mathbb{C} \setminus \Xi_\alpha\,, \tag{11.8}$$

where $\|\cdot\|$ denotes the operator norm in $L^2(\Omega)$.

Given a closed operator H in a Hilbert space $\mathcal{H}$, we use the following decomposition of the spectrum $\sigma(H)$:

Definition 11.1. The *point* spectrum $\sigma_{\mathrm{p}}(H)$ equals the set of points λ such that $H - \lambda$ is not injective. The *essential* spectrum $\sigma_{\mathrm{e}}(H)$ equals the set of points λ such that $H - \lambda$ is not Fredholm. Finally, the *residual* spectrum $\sigma_{\mathrm{r}}(H)$ equals the set of points λ such that $H - \lambda$ is injective but the range of $H - \lambda$ is not dense in $\mathcal{H}$.

Remark 11.1. 1. The reader is warned that various other types of essential spectra of non-self-adjoint operators are used in the literature; *cf* [11, Chapt. IX] for five distinct definitions and a detailed description of their properties. Among them we choose that of Wolf [27], which is in general larger than that of Kato [18, Sec. IV.5.6] based on violating the semi-Fredholm property. (Recall that a closed operator in a Hilbert space is called Fredholm if its range is closed and both its kernel and its cokernel are finite-dimensional, while it is called semi-Fredholm if its range is closed and its kernel or its cokernel is finite-dimensional.) However, since our operator H_α is $\mathcal{T}$-self-adjoint, the majority of the different definitions coincide [11, Thm IX.1.6], in particular the two above, and that is why we use the common notation $\sigma_{\mathrm{e}}(\cdot)$ in this paper. Then our choice also coincides with the definition of "continuous spectrum" as used for instance in the Glazman's book [14].

2. We indeed have the decomposition (*cf* [14, Sec. I.1.1])

$$\sigma(H) = \sigma_{\mathrm{p}}(H) \cup \sigma_{\mathrm{e}}(H) \cup \sigma_{\mathrm{r}}(H)\,,$$

but note that there might be intersections on the right hand side. In particular, $\sigma_{\mathrm{e}}(H)$ contains eigenvalues of infinite geometric multiplicity.

3. On the other hand, the definitions of point and residual spectra are standard and they form disjoint subsets of $\sigma(H)$. Recalling the general fact [18, Sec. V.3.1] that the orthogonal complement of the range of a densely defined closed operator in a Hilbert space is equal to the kernel of its adjoint, we obtain the following characterization of the residual spectrum in terms of the point spectrum of the operator and its adjoint:

$$\sigma_{\mathrm{r}}(H) = \left\{ \lambda \in \mathbb{C} \mid \bar{\lambda} \in \sigma_{\mathrm{p}}(H^*) \;\&\; \lambda \notin \sigma_{\mathrm{p}}(H) \right\}. \tag{11.9}$$

The $\mathcal{T}$-self-adjointness of H_α immediately implies:

Corollary 11.1. *Suppose the hypothesis of Theorem 11.1. Then*

$$\sigma_{\mathrm{r}}(H_\alpha) = \varnothing\,.$$

Proof. We repeat the proof sketched in Introduction. Since H_α is $\mathcal{T}$-self-adjoint, it is easy to see that λ is an eigenvalue of H_α (with eigenfunction Ψ) if, and only if, $\bar{\lambda}$ is an eigenvalue of H_α^* (with eigenfunction $\overline{\Psi}$). It is then clear from the general identity (11.9) that the residual spectrum of H_α must be empty. $\square$

The case of uniform boundary conditions, *i.e.* when α equals identically a constant α_0, can be solved by separation of variables (*cf* Section 11.4). We find

$$\sigma(H_{\alpha_0}) = \sigma_{\mathrm{e}}(H_{\alpha_0}) = [\mu_0^2, +\infty)\,, \tag{11.10}$$

where the threshold μ_0^2, with the notation

$$\mu_0 = \begin{cases} \alpha_0 & \text{if} \quad |\alpha_0| \leqslant \pi/d\,, \\ \pi/d & \text{if} \quad |\alpha_0| > \pi/d\,, \end{cases} \tag{11.11}$$

denotes the bottom of the spectrum of the "transverse" operator

$$\begin{aligned} -\Delta_{\alpha_0}^I \psi &:= -\psi'', \\ \psi \in \mathsf{D}(-\Delta_{\alpha_0}^I) &:= \left\{\psi \in W_2^2(I) \mid \psi' + \mathrm{i}\alpha_0\psi = 0 \quad \text{at} \quad \partial I\right\}. \end{aligned} \tag{11.12}$$

The operator $-\Delta_{\alpha_0}^I$ was studied in [20]. Its spectrum is purely discrete and real:

$$\sigma(-\Delta_{\alpha_0}^I) = \{\mu_j^2\}_{j=0}^{\infty}\,, \tag{11.13}$$

where μ_0 has been introduced in (11.11),

$$\mu_1 = \begin{cases} \alpha_0 & \text{if} \quad |\alpha_0| > \pi/d\,, \\ \pi/d & \text{if} \quad |\alpha_0| \leqslant \pi/d\,, \end{cases} \qquad \text{and} \qquad \mu_j := \pi j/d \quad \text{for} \quad j \geqslant 2\,.$$

Making the hypothesis

$$\alpha_0 d/\pi \;\notin\; \mathbb{Z}\backslash\{0\}\,, \tag{11.14}$$

the eigenvalues of $-\Delta_{\alpha_0}^I$ are simple and the corresponding set of eigenfunctions $\{\psi_j\}_{j=0}^{\infty}$ can be chosen as

$$\psi_j(x_2) := \cos(\mu_j x_2) - \mathrm{i}\,\frac{\alpha_0}{\mu_j}\,\sin(\mu_j x_2)\,. \tag{11.15}$$

We refer to Section 11.4.1 for more results about the operator $-\Delta_{\alpha_0}^I$.

Let us now turn to the non-trivial case of variable coupling function α. Among a variety of possible situations, in this paper we restrict the considerations to local perturbations of the uniform case. Namely, we always assume that the difference $\alpha - \alpha_0$ is compactly supported.

First of all, in Section 11.5 we show that the essential component of the spectrum of H_α is stable under the local perturbation of the uniform case:

Theorem 11.2. *Let $\alpha - \alpha_0 \in C_0(\mathbb{R}) \cap W_\infty^1(\mathbb{R})$ with $\alpha_0 \in \mathbb{R}$. Then*

$$\sigma_{\mathrm{e}}(H_\alpha) = [\mu_0^2, +\infty)\,.$$

Notice that the essential spectrum as a set is independent of α_0 as long as $|\alpha_0| \geqslant \pi/d$. This is a consequence of the fact that our Hamiltonian is not Hermitian. On the other hand, it follows that the essential spectrum is real. Recall that the residual spectrum is always empty due to Corollary 11.1. We do not have the proof of the reality for the point spectrum, except for the particular case treated in the next statement:

Theorem 11.3. *Let $\alpha \in C_0(\mathbb{R}) \cap W_\infty^1(\mathbb{R})$ be an odd function. Then*

$$\sigma_{\mathrm{p}}(H_\alpha) \subset \mathbb{R}\,.$$

Summing up, under the hypotheses of this theorem the total spectrum is real (and in fact non-negative due to (11.7)).

The next part of our results concerns the behavior of the point spectrum of H_α under a small perturbation of α_0. Namely, we consider the local perturbation of the form

$$\alpha(x_1) = \alpha_0 + \varepsilon\,\beta(x_1)\,, \tag{11.16}$$

where $\beta \in C_0^2(\mathbb{R})$ and ε is a small positive parameter. In accordance with Theorem 11.2, in this case the essential spectrum of H_α coincides with $[\mu_0^2, +\infty)$, and this is also the spectrum of H_{α_0}. Our main interest is focused on the existence and asymptotic behavior of the eigenvalues emerging from the threshold μ_0^2 due to the perturbation of H_{α_0} by $\varepsilon\beta$.

First we show that the asymtotically Neumann case is in some sense exceptional:

Theorem 11.4. *Suppose $\alpha_0 = 0$. Let α be given by* (11.16)*, where $\beta \in C_0^2(\mathbb{R})$. Then the operator H_α has no eigenvalues converging to μ_0^2 as $\varepsilon \to +0$.*

The problem of existence of the weakly-coupled eigenvalues is more subtle as long as $\alpha_0 \neq 0$. To present our results in this case, we introduce an auxiliary sequence of functions $v_j : \mathbb{R} \to \mathbb{R}$ by

$$v_j(x_1) := \begin{cases} -\dfrac{1}{2}\displaystyle\int_{\mathbb{R}} |x_1 - t_1|\beta(t_1)\,\mathrm{d}t_1 & \text{if} \quad j = 0\,, \\ \dfrac{1}{2\sqrt{\mu_j^2 - \mu_0^2}}\displaystyle\int_{\mathbb{R}} \mathrm{e}^{-\sqrt{\mu_j^2-\mu_0^2}|x_1-t_1|}\beta(t_1)\,\mathrm{d}t_1 & \text{if} \quad j \geqslant 1\,. \end{cases} \tag{11.17}$$

Denoting $\langle f\rangle = \int_{\mathbb{R}} f(x_1)\,\mathrm{d}x_1$ for any $f \in L_1(\mathbb{R})$, we introduce a constant τ, depending on β, d and α_0, by

$$\tau := \begin{cases} 2\alpha_0^2\langle\beta v_0\rangle + \dfrac{2\alpha_0}{d}\displaystyle\sum_{j=1}^{\infty}\frac{\mu_j^2\langle\beta v_j\rangle}{\mu_j^2-\mu_0^2}\tan\frac{\alpha_0 d + j\pi}{2} & \text{if} \quad |\alpha_0| < \dfrac{\pi}{d}\,, \\ \dfrac{2\alpha_0\pi^2\cot\frac{\alpha_0 d}{2}}{(\mu_1^2-\mu_0^2)d^3}\langle\beta v_1\rangle + \dfrac{8\pi^2}{(\mu_1^2-\mu_0^2)d^4}\displaystyle\sum_{j=1}^{\infty}\frac{\mu_{2j}^2\langle\beta v_{2j}\rangle}{\mu_{2j}^2-\mu_1^2} & \text{if} \quad |\alpha_0| > \dfrac{\pi}{d}\,. \end{cases}$$

It will be shown in Section 11.6.3 that the series converge. Finally, we denote $\Omega_a := \Omega \cap \{x : |x_1| < a\}$ for any positive a. Now we are in a position to state our main results about the point spectrum.

Theorem 11.5. *Suppose $|\alpha_0| < \pi/d$. Let α be given by* (11.16)*, where $\beta \in C_0^2(\mathbb{R})$.*

1. *If $\alpha_0\langle\beta\rangle < 0$, there exists the unique eigenvalue λ_ε of H_α converging to μ_0^2 as $\varepsilon \to +0$. This eigenvalue is simple and real, and satisfies the asymptotic formula*
$$\lambda_\varepsilon = \mu_0^2 - \varepsilon^2\alpha_0^2\langle\beta\rangle^2 + 2\varepsilon^3\alpha_0\tau\langle\beta\rangle + \mathcal{O}(\varepsilon^4)\,.$$
The associated eigenfunction Ψ_ε can be chosen so that it satisfies the asymptotics
$$\Psi_\varepsilon(x) = \psi_0(x_2) + \mathcal{O}(\varepsilon) \tag{11.18}$$
in $W_2^2(\Omega_a)$ for each $a > 0$, and behaves at infinity as
$$\Psi_\varepsilon(x) = \mathrm{e}^{-\sqrt{\mu_0^2-\lambda_\varepsilon}|x_1|}\psi_0(x_2) + \mathcal{O}(\mathrm{e}^{-\sqrt{\mu_0^2-\lambda_\varepsilon}|x_1|})\,, \quad |x_1| \to +\infty\,. \tag{11.19}$$

2. *If $\alpha_0\langle\beta\rangle > 0$, the operator H_α has no eigenvalues converging to μ_0^2 as $\varepsilon \to +0$.*

3. *If $\langle\beta\rangle = 0$, and $\tau > 0$, there exists the unique eigenvalue λ_ε of H_α converging to μ_0^2 as $\varepsilon \to +0$. This eigenvalue is simple and real, and satisfies the asymptotics*
$$\lambda_\varepsilon = \mu_0^2 - \varepsilon^4\tau^2 + \mathcal{O}(\varepsilon^5)\,. \tag{11.20}$$
The associated eigenfunction can be chosen so that the relations (11.18) *and* (11.19) *hold true.*

4. *If $\langle\beta\rangle = 0$, and $\tau < 0$, the operator H_α has no eigenvalues converging to μ_0^2 as $\varepsilon \to +0$.*

Theorem 11.6. *Suppose $|\alpha_0| > \pi/d$ and* (11.14)*. Let α be given by* (11.16) *where $\beta \in C_0^2(\mathbb{R})$.*

1. *If $\tau > 0$, there exists the unique eigenvalue λ_ε of H_α converging to μ_0 as $\varepsilon \to +0$, it is simple and real, and satisfies the asymptotics* (11.20)*. The associated eigenfunction can be chosen so that it obeys* (11.18) *and* (11.19)*.*

2. *If $\tau < 0$, the operator H_α has no eigenvalues converging to μ_0^2 as $\varepsilon \to +0$.*

In accordance with Theorem 11.5, in the case $|\alpha_0| < \pi/d$ the existence of a weakly-coupled eigenvalue is determined by the sign of the constant α_0 and that of the mean value of β. In the language of Schrödinger operators (treating α as a singular potential), it means that a given non-trivial β plays the role of an effective interaction, attractive or repulsive depending upon the sign of α_0. It is instructive to compare this situation with a self-adjoint waveguide [6], where a similar effective interaction is induced by a local deformation of the boundary. If the boundary is deformed “outward in the mean”, a weakly-coupled bound state exists, while it is absent if the deformation is “inward-pointing in the mean”.

As usual, the critical situation $\langle\beta\rangle = 0$ is much harder to treat. In our case, one has to check the sign of τ to decide whether a weakly-coupled bound state exists. However, it can be difficult to sum up the series in the definition of τ. This is why in our next statement we provide a sufficient condition guaranteeing that $\tau > 0$.

Proposition 11.1. *Suppose* $0 < |\alpha_0| < \pi/d$. *Let* α *be given by* (11.16) *where* $\beta(x_1) = \widetilde{\beta}(x_1/l)$, $\widetilde{\beta} \in C_0^2(\mathbb{R})$, $\langle\widetilde{\beta}\rangle = 0$, $l > 0$. *If*

$$\left\| \int_{\mathbb{R}} \operatorname{sgn}(\cdot - t_1)\widetilde{\beta}(t_1)\, \mathrm{d}t_1 \right\|^2_{L_2(\mathbb{R})} \geqslant \frac{4\cot\frac{\alpha_0 d}{2}}{l^2\,\alpha_0 d} \left[\frac{\mu_1^2}{(\mu_1^2 - \mu_0^2)^2} + \frac{d^2}{16\pi^2} + \frac{d^2}{48} \right] \|\widetilde{\beta}\|^2_{L_2(\mathbb{R})}\,,$$

then $\tau > 0$.

The meaning of this proposition is that for each positive $|\alpha_0| < \pi/d$ the perturbation $\varepsilon\beta$ in the critical regime $\langle\beta\rangle = 0$ produces a weakly-coupled eigenvalue near the threshold of the essential spectrum provided that the support of β is wide enough. This is in perfect agreement with the critical situation of [6]; according to higher-order asymptotics derived in [5], here the weakly-coupled bound state exists if, and only if, the critical boundary deformation is smeared enough.

In the case $|\alpha_0| > \pi/d$ a sufficient condition guaranteeing $\tau > 0$ is given in

Proposition 11.2. *Suppose* $|\alpha_0| > \pi/d$ *and* (11.14). *Let* α *be given by* (11.16) *where* $\beta \in C_0^2(\mathbb{R})$. *Let* m *be the maximal positive integer such that* $\mu_{2m} < |\alpha_0|$. *If*

$$\alpha_0\langle\beta v_1\rangle \cot\frac{\alpha_0 d}{2} \geqslant \frac{4}{d}\sum_{j=1}^{m} \frac{\mu_{2j}^2\langle\beta v_{2j}\rangle}{\mu_1^2 - \mu_{2j}^2}\,, \tag{11.21}$$

then $\tau > 0$.

In Section 11.6.6 we will show that the inequality (11.21) makes sense. Namely, it will be proved that there exists β such that this inequality holds true, provided that α_0 is close enough to μ_2 but greater than this value.

Remark 11.2. It is useful to make the hypothesis (11.14), since it implies that the "transverse" eigenfunctions (11.15) form a basis (*cf* (11.24)) and makes it therefore possible to obtain a relatively simple decomposition of the resolvent of H_{α_0} (*cf* Lemma 11.5). However, it is rather a technical hypothesis for many of the spectral results (*e.g.*, Theorem 11.2). On the other hand, it seems that the hypothesis is rather crucial for the statement of Theorem 11.6 and Proposition 11.2.

If the hypothesis (11.14) is omitted and $\alpha_0 = \pi\ell/d$, with $\ell \in \mathbb{Z}\setminus\{0\}$, the threshold of the essential spectrum is π^2/d^2. This point corresponds to a simple eigenvalue of the "transverse" operator $-\Delta^I_{\alpha_0}$ only if $|\ell| > 1$, while it is a double eigenvalue if $|\ell| = 1$. Under the hypothesis of Theorems 11.5 and 11.6, the threshold is always a simple eigenvalue of $-\Delta^I_{\alpha_0}$, and the proof of the theorems actually employs some sort of "non-degenerate" perturbation theory. In view of this, we conjecture that in the degenerate case $|\ell| = 1$ two simple eigenvalues (possibly forming a complex conjugate pair) or one double (real) eigenvalue can emerge from the threshold of the essential spectrum for a suitable choice of β, while in the case $|\ell| > 1$ there can be at most one simple emerging eigenvalue. The question on the asymptotic behaviour of these eigenvalues constitutes an interesting open problem.

11.3 Definition of the operator

In this section we prove Theorem 11.1. Our method is based on the theory of sectorial sesquilinear forms [18, Sec. VI].

In the beginning we assume only that α is bounded. Let h_α be the sesquilinear form defined in $L^2(\Omega)$ by the domain $\mathsf{D}(h_\alpha) := W_2^1(\Omega)$ and the prescription $h_\alpha := h_\alpha^1 + \mathrm{i}h_\alpha^2$ with

$$\begin{aligned} h_\alpha^1(\Psi,\Phi) &:= \int_\Omega \nabla\Psi(x)\cdot\overline{\nabla\Phi(x)}\,dx\,,\\ h_\alpha^2(\Psi,\Phi) &:= \int_{\mathbb{R}} \alpha(x_1)\,\Psi(x_1,d)\,\overline{\Phi(x_1,d)}\,dx_1 - \int_{\mathbb{R}} \alpha(x_1)\,\Psi(x_1,0)\,\overline{\Phi(x_1,0)}\,dx_1\,, \end{aligned}$$

for any $\Psi,\Phi \in \mathsf{D}(h_\alpha)$. Here the dot denotes the scalar product in $\mathbb{R}^2$ and the boundary terms should be understood in the sense of traces [1]. We write $h_\alpha[\Psi] := h_\alpha(\Psi,\Psi)$ for the associated quadratic form, and similarly for h_α^1 and h_α^2.

Clearly, h_α is densely defined. It is also clear that the real part h_α^1 is a densely defined, symmetric, positive, closed sesquilinear form (it is associated to the self-adjoint Neumann Laplacian in $L^2(\Omega)$). Of course, h_α itself is not symmetric unless α vanishes identically; however, it can be shown that it is sectorial and closed. To see it, one can use the perturbation result [18, Thm. VI.1.33] stating that the sum of a sectorial closed form with a relatively bounded form is sectorial and closed provided the relative bound is less than one. In our case, the imaginary part h_α^2 plays the role of the small perturbation of h_α^1 by virtue of the following result.

Lemma 11.1. *Let $\alpha \in L^\infty(\mathbb{R})$. Then h_α^2 is relatively bounded with respect to h_α^1, with*

$$\left|h_\alpha^2[\Psi]\right| \leqslant 2\,\|\alpha\|_{L^\infty(\mathbb{R})}\,\|\Psi\|_{L^2(\Omega)}\sqrt{h_\alpha^1[\Psi]} \leqslant \delta\, h_\alpha^1[\Psi] + \delta^{-1}\,\|\alpha\|^2_{L^\infty(\mathbb{R})}\,\|\Psi\|^2_{L^2(\Omega)}$$

for all $\Psi \in W_2^1(\Omega)$ and any positive number δ.

Proof. By density [1, Thm. 3.18], it is sufficient to prove the inequality for restrictions to Ω of functions Ψ in $C_0^\infty(\mathbb{R}^2)$. Then we have

$$\left|h_\alpha^2[\Psi]\right| = \left|\int_\Omega \alpha(x_1)\,\frac{\partial|\Psi(x)|^2}{\partial x_2}\,dx\right| \leqslant 2\,\|\alpha\|_{L^\infty(\mathbb{R})}\,\|\Psi\|_{L^2(\Omega)}\,\|\partial_2\Psi\|_{L^2(\Omega)}\,,$$

which gives the first inequality after applying $\|\partial_2\Psi\|_{L^2(\Omega)} \leqslant \|\nabla\Psi\|_{L^2(\Omega)}$. The second inequality then follows at once by means of the Cauchy inequality with δ. ☐

In view of the above properties, Theorem VI.1.33 in [18], and the first representation theorem [18, Thm. VI.2.1], there exists the unique m-sectorial operator $\tilde{H}_\alpha$ in $L^2(\Omega)$ such that $h_\alpha(\Psi,\Phi) = (\tilde{H}_\alpha\Psi,\Phi)$ for all $\Psi \in \mathsf{D}(\tilde{H}_\alpha) \subset \mathsf{D}(h_\alpha)$ and $\Phi \in \mathsf{D}(h_\alpha)$, where

$$\mathsf{D}(\tilde{H}_\alpha) = \left\{\Psi \in W_2^1(\Omega) \,|\, \exists F \in L^2(\Omega),\ \forall \Phi \in W_2^1(\Omega),\ h_\alpha(\Psi,\Phi) = (F,\Phi)_{L^2(\Omega)}\right\}.$$

By integration by parts, it is easy to check that if $\Psi \in \mathsf{D}(H_\alpha)$, it follows that $\Psi \in \mathsf{D}(\tilde{H}_\alpha)$ with $F = -\Delta\Psi$. That is, $\tilde{H}_\alpha$ is an extension of H_α as defined in (11.4). It remains to show that actually $H_\alpha = \tilde{H}_\alpha$ in order to prove Theorem 11.1. However, the other inclusion holds as a direct consequence of the representation theorem and the following result.

Lemma 11.2. *Let $\alpha \in W_\infty^1(\mathbb{R})$. For each $F \in L_2(\Omega)$, a generalized solution Ψ to the problem*

$$\begin{cases} -\Delta\Psi = F & \text{in } \Omega\,, \\ \partial_2\Psi + \mathrm{i}\,\alpha\,\Psi = 0 & \text{on } \partial\Omega\,, \end{cases} \tag{11.22}$$

belongs to $\mathsf{D}(H_\alpha)$.

Proof. For any function $\Psi \in W_2^1(\Omega)$, we introduce the difference quotient

$$\Psi_\delta(x) := \frac{\Psi(x_1+\delta,x_2) - \Psi(x)}{\delta}\,,$$

where δ is a small real number. By standard arguments [23, Ch. III, Sec. 3.4, Thm. 3], the estimate

$$\|\Psi_\delta\|_{L_2(\Omega)} \leqslant \|\Psi\|_{W_2^1(\Omega)} \tag{11.23}$$

holds true for all δ small enough. If Ψ is a generalized solution to (11.22), then Ψ_δ is a generalized solution to the problem

$$\begin{cases} -\Delta\Psi_\delta = F_\delta & \text{in } \Omega\,, \\ \partial_2\Psi_\delta + \mathrm{i}\,\alpha\,\Psi_\delta = g & \text{on } \partial\Omega\,, \end{cases}$$

where g denotes the trace of the function $x \mapsto -\mathrm{i}\alpha_\delta(x_1)\Psi(x_1+\delta,x_2)$ to the boundary $\partial\Omega$. Using the "integration-by-parts" formula for the difference quotients, $(F_\delta,\Phi)_{L_2(\Omega)} = -(F,\Phi_{-\delta})_{L_2(\Omega)}$, the integral identity corresponding to the weak formulation of the boundary value problem for Ψ_δ can be written as follows

$$h_\alpha(\Psi_\delta,\Phi) = -(F,\Phi_{-\delta})_{L_2(\Omega)} - \mathrm{i}\int_{\mathbb{R}} \alpha_\delta(x_1)\,\Psi(x_1+\delta,d)\,\overline{\Phi(x_1,d)}\,dx_1 \\ + \mathrm{i}\int_{\mathbb{R}} \alpha_\delta(x_1)\,\Psi(x_1+\delta,0)\,\overline{\Phi(x_1,0)}\,dx_1\,,$$

where $\Phi \in W_2^1(\Omega)$ is arbitrary. Letting $\Phi = \Psi_\delta$, and using the embedding of $W_2^1(\Omega)$ in $L_2(\partial\Omega)$, the boundedness of α_δ, Lemma 11.1 and (11.23), the above identity yields

$$\|\Psi_\delta\|_{W_2^1(\Omega)} \leqslant C\,,$$

where the constant C is independent of δ. Employing this estimate and proceeding as in the proof of Item b) of Theorem 3 in [23, Ch. III, Sec. 3.4], one can show easily that $\partial_1\Psi \in W_2^1(\Omega)$. Hence, $\partial_{11}\Psi \in L_2(\Omega)$ and $\partial_{12}\Psi \in L_2(\Omega)$.

If follows from standard elliptic regularity theorems (see, *e.g.*, [23, Ch. IV, Sec. 2.2]) that $\Psi \in W^2_{2,loc}(\Omega)$. Hence, the first of the equations in (11.22) holds true a.e. in Ω. Thus, $\partial_{22}\Psi = -F - \partial_{11}\Psi \in L_2(\Omega)$, and therefore $\Psi \in W^2_2(\Omega)$.

It remains to check the boundary condition for Ψ. Integrating by parts, one has

$$\begin{aligned}(F,\Phi)_{L^2(\Omega)} =& h_\alpha(\Psi,\Phi) = (-\Delta\Psi,\Phi)_{L_2(\Omega)} \\ &+ \int_{\mathbb{R}} \left[\partial_2\Psi(x_1,d) + \mathrm{i}\,\alpha(x_1)\,\Psi(x_1,d)\right] \overline{\Phi(x_1,d)}\,dx_1 \\ &- \int_{\mathbb{R}} \left[\partial_2\Psi(x_1,0) + \mathrm{i}\,\alpha(x_1)\,\Psi(x_1,0)\right] \overline{\Phi(x_1,0)}\,dx_1\end{aligned}$$

for any $\Phi \in W^1_2(\Omega)$. This implies the boundary conditions because $-\Delta\Psi = F$ a.e. in Ω and Φ is arbitrary. □

Summing up the results of this section, we get

Proposition 11.3. *Let $\alpha \in W^1_\infty(\mathbb{R})$. Then $\tilde{H}_\alpha = H_\alpha$.*

Theorem 11.1 follows as a corollary of this proposition. In particular, the latter implies that H_α is m-sectorial. Moreover, by the first representation theorem, we know that the adjoint $\tilde{H}^*_\alpha$ is simply obtained as the operator associated with $h^*_\alpha = h_{-\alpha}$. This together with Proposition 11.3 proves (11.5).

Let us finally comment on the results (11.7) and (11.8). As a direct consequence of the first inequality of Lemma 11.2, we get that the numerical range of $H_\alpha (= \tilde{H}_\alpha)$, defined as the set of all complex numbers $(H_\alpha\Psi,\Psi)_{L^2(\Omega)}$ where Ψ changes over all $\Psi \in \mathsf{D}(H_\alpha)$ with $\|\Psi\|_{L^2(\Omega)} = 1$, is contained in the set Ξ_α. Hence, in view of general results about numerical range (*cf* [18, Sec. V.3.2]), the exterior of the numerical range of H_α is a connected set, and one indeed has (11.7) and (11.8).

11.4 The unperturbed waveguide

In this section we consider the case of uniform boundary conditions in the sense that α is supposed to be identically equal to a constant $\alpha_0 \in \mathbb{R}$. We prove the spectral result (11.10) by using the fact that H_{α_0} can be decomposed into a sum of the "longitudinal" operator $-\Delta^{\mathbb{R}}$, *i.e.* the self-adjoint Laplacian in $L^2(\mathbb{R})$, and the "transversal" operator $-\Delta^I_{\alpha_0}$ defined in (11.12).

11.4.1 The transversal operator

We summarize here some of the results established in [20] and refer to that reference for more details.

The adjoint of $-\Delta^I_{\alpha_0}$ is simply obtained by the replacement $\alpha_0 \mapsto -\alpha_0$, *i.e.*, $(-\Delta^I_{\alpha_0})^* = -\Delta^I_{-\alpha_0}$. Consequently, $(-\Delta^I_{\alpha_0})^*$ has the same spectrum (11.13) and the corresponding set of eigenfunctions $\{\phi_j\}_{j=0}^\infty$ can be chosen as

$$\phi_j(x_2) := \overline{A_j\,\psi_j(x_2)}\,,$$

where $\{\psi_j\}_{j=0}^\infty$ have been introduced in (11.15) and A_j are normalization constants. Choosing

$$A_{j_0} := \frac{2\mathrm{i}\alpha_0}{1-\exp\left(-2\mathrm{i}\alpha_0 d\right)}\,, \quad A_{j_1} := \frac{2\mu_1^2}{(\mu_1^2-\alpha_0^2)d}\,, \quad A_j := \frac{2\mu_j^2}{(\mu_j^2-\alpha_0^2)d}\,,$$

where $j \geqslant 2$, $(j_0,j_1) = (0,1)$ if $|\alpha_0| < \pi/d$ and $(j_0,j_1) = (1,0)$ if $|\alpha_0| > \pi/d$ (if $\alpha_0 = 0$, the fraction in the definition of A_{j_0} should be understood as the expression obtained after taking the limit $\alpha_0 \to 0$), we have the biorthonormality relations

$$\forall j,k \in \mathbb{N}, \quad (\psi_j,\phi_k)_{L^2(I)} = \delta_{jk}$$

together with the biorthonormal-basis-type expansion (*cf* [20, Prop. 4])

$$\forall \psi \in L^2(I)\,, \qquad \psi = \sum_{j=0}^\infty (\psi,\phi_j)_{L^2(I)}\,\psi_j\,. \tag{11.24}$$

Let us show that (11.24) can be extended to $L^2(\Omega)$.

Lemma 11.3. *For any $\Psi \in L_2(\Omega)$, the identity*

$$\Psi(x) = \sum_{j=0}^\infty \Psi_j(x_1)\,\psi_j(x_2) \qquad \text{with} \qquad \Psi_j(x_1) := \big(\Psi(x_1,\cdot),\phi_j\big)_{L_2(I)}$$

holds true in the sense of $L_2(\Omega)$-norm.

Proof. In view of (11.24), the series converges to Ψ in $L^2(I)$ for almost every $x_1 \in \mathbb{R}$. We use the dominated convergence theorem to prove that the convergence actually holds in the norm of $L^2(\Omega)$. To do so, it is sufficient to check that the $L^2(I)$-norm of the partial sums can be uniformly estimated by a function from $L^2(\mathbb{R})$.

Let us introduce $\chi_j^D(x_2) := \sin(\pi j x_2/d)$ and $\chi_j^N(x_2) := \cos(\pi j x_2/d)$ for $j \geqslant 1$, and $\chi_0^N(x_2) := 1/\sqrt{2}$. We recall that $\{\sqrt{2/d}\,\chi_j^D\}_{j=1}^\infty$ and $\{\sqrt{2/d}\,\chi_j^N\}_{j=0}^\infty$ form complete orthonormal families in $L^2(I)$. Expressing ψ_j in terms of χ_j^N and χ_j^D for $j \geqslant 2$, and using the orthonormality, we have ($n \geqslant 2$)

$$\begin{aligned}\Big\|\sum_{j=2}^n \Psi_j(x_1)\,\psi_j\Big\|_{L_2(I)}^2 &\leqslant d\Big\|\sum_{j=2}^n \Psi_j(x_1)\,\chi_j^N\Big\|_{L_2(I)}^2 + d\,\alpha_0^2\Big\|\sum_{j=2}^n \Psi_j(x_1)\,\chi_j^D/\mu_j\Big\|_{L_2(I)}^2 \\ &= d\sum_{j=2}^n |\Psi_j(x_1)|^2 + d\,\alpha_0^2\sum_{j=2}^n |\Psi_j(x_1)|^2/\mu_j^2 \\ &\leqslant d\left(1+\frac{\alpha_0^2}{\mu_2^2}\right)\sum_{j=2}^\infty |\Psi_j(x_1)|^2 \,. \end{aligned} \tag{11.25}$$

Next, writing ($j \geqslant 2$)

$$\Psi_j = \sqrt{\frac{d}{2}}\,A_j\left(\Psi_j^N - \mathrm{i}\frac{\alpha_0}{\mu_j}\,\Psi_j^D\right) \qquad \text{with} \qquad \Psi_j^\sharp(x_1) := \big(\Psi(x_1,\cdot),\chi_j^\sharp\big)_{L_2(I)}\,,$$

noticing that $|A_j| \leqslant c$ (valid for all $j \geqslant 0$) where c is a constant depending uniquely on $|\alpha_0|$ and d, and using the Parseval identities for χ_j^N and χ_j^D, we obtain

$$\begin{aligned}\sum_{j=2}^\infty |\Psi_j(x_1)|^2 &\leqslant c^2 d\sum_{j=2}^\infty\left(|\Psi_j^N|^2 + \frac{\alpha_0^2}{\mu_j^2}\,|\Psi_j^D|^2\right) \\ &\leqslant c^2 d\left(1+\frac{\alpha_0^2}{\mu_2^2}\right)\|\Psi(x_1,\cdot)\|_{L_2(I)}^2\,. \end{aligned} \tag{11.26}$$

At the same time, using just the estimates $|\psi_j|^2 \leqslant (1+\alpha_0^2/\mu_j^2)$ valid for all $j \geqslant 0$, we readily get

$$\Big\|\sum_{j=0}^1 \Psi_j(x_1)\,\psi_j\Big\|_{L_2(I)} \leqslant 2\,c\,d\left(1+\frac{\alpha_0^2}{\mu_0^2}\right)\|\Psi(x_1,\cdot)\|_{L_2(I)}\,. \tag{11.27}$$

Summing up,

$$\Big\|\sum_{j=0}^n \Psi_j(x_1)\,\psi_j\Big\|_{L_2(I)} \leqslant C\,\|\Psi(x_1,\cdot)\|_{L_2(I)} \in L_2(\mathbb{R})\,,$$

where C is a constant independent of n, and the usage of the dominated convergence theorem is justified. □

11.4.2 Spectrum of the unperturbed waveguide

First we show that the spectrum of H_{α_0} is purely essential. Since the residual spectrum is always empty due to Corollary 11.1, it is enough to show that there are no eigenvalues.

Proposition 11.4. *Let* $\alpha_0 \in \mathbb{R}$ *satisfy* (11.14). *Then*

$$\sigma_{\mathrm{p}}(H_{\alpha_0}) = \varnothing\,.$$

Proof. Suppose that H_{α_0} possesses an eigenvalue λ with eigenfunction Ψ. Multiplying the eigenvalue equation with $\overline{\phi_j}$ and integrating over I, we arrive at the equations

$$-\Psi_j'' = (\lambda-\mu_j^2)\Psi_j \qquad \text{in} \qquad \mathbb{R}\,, \qquad j \geqslant 0\,,$$

where Ψ_j are the coefficients of Lemma 11.3. Since $\Psi_j \in L^2(\mathbb{R})$ due to Fubini's theorem, each of the equations has just a trivial solution. This together with Lemma 11.3 yields $\Psi = 0$, a contradiction. That is, the point spectrum of H_{α_0} is empty. □

Remark 11.3. Regardless of the technical hypothesis (11.14), the set of isolated eigenvalues of H_{α_0} is always empty. This follows from Proposition 11.4 and the fact that $\alpha_0 \mapsto H_{\alpha_0}$ forms a holomorphic family of operators [18, Sec. VII.4].

It is well known that the spectrum of the "longitudinal" operator $-\Delta^{\mathbb{R}}$ is also purely essential and equal to the semi-axis $[0,+\infty)$. In view of the separation of variables, it is reasonable to expect that the (essential) spectrum of H_{α_0} will be given by that semi-axis shifted by the first eigenvalue of $-\Delta^I_{\alpha_0}$. First we show that the resulting interval indeed belongs to the spectrum of H_{α_0}.

Lemma 11.4. *Let* $\alpha_0 \in \mathbb{R}$*. Then* $[\mu_0^2,+\infty) \subseteq \sigma_{\mathrm{e}}(H_{\alpha_0})$*.*

Proof. Since the spectrum of H_{α_0} is purely essential, it can be characterized by means of singular sequences [11, Thm. IX.1.3] (it is in fact an equivalent definition of another type of essential spectrum, which is in general intermediate between the essential spectra due to Wolf and Kato, and therefore coinciding with them in our case, *cf* Remark 11.1). That is, $\lambda \in \sigma_{\mathrm{e}}(H_{\alpha_0})$ if, and only if, there exists a sequence $\{u_n\}_{n=1}^\infty \subset \mathsf{D}(H_{\alpha_0})$ such that $\|u_n\|_{L^2(\Omega)} = 1$, $u_n \rightharpoonup 0$ and $\|H_{\alpha_0}u_n - \lambda u_n\|_{L^2(\Omega)} \to 0$ as $n \to \infty$. Let $\{\varphi_n\}_{n=1}^\infty$ be a singular sequence of $-\Delta^{\mathbb{R}}$ corresponding to a given $z \in [0,+\infty)$. Then it is easy to verify that u_n defined by $u_n(x) := \varphi_n(x_1)\psi_0(x_2)/\|\psi_0\|_{L^2(I)}$ forms a singular sequence of H_{α_0} corresponding to $z+\mu_0^2$. □

To get the opposite inclusion, we employ the fact that the biorthonormal-basis-type relations (11.24) are available. This enables us to decompose the resolvent of H_{α_0} into the transverse biorthonormal-basis.

Lemma 11.5. *Let* $\alpha_0 \in \mathbb{R}$ *satisfy* (11.14)*. Then* $\mathbb{C}\setminus[\mu_0^2,+\infty) \subseteq \rho(H_{\alpha_0})$ *and for any* $z \in \mathbb{C}\setminus[\mu_0^2,+\infty)$ *we have*

$$(H_{\alpha_0}-z)^{-1} = \sum_{j=0}^{\infty}(-\Delta^{\mathbb{R}}+\mu_j^2-z)^{-1}B_j\,.$$

Here B_j *is a bounded operator on* $L^2(\Omega)$ *defined by*

$$(B_j\Psi)(x) := \big(\Psi(x_1,\cdot),\phi_j\big)_{L^2(I)}\,\psi_j(x_2)\,, \qquad \Psi \in L^2(\Omega)\,,$$

and $(-\Delta^{\mathbb{R}}+\mu_j^2-z)^{-1}$ *abbreviates* $(-\Delta^{\mathbb{R}}+\mu_j^2-z)^{-1}\otimes 1$ *on* $L^2(\mathbb{R})\otimes L^2(I) \simeq L^2(\Omega)$*.*

Proof. Put $z \in \mathbb{C}\setminus[\mu_0^2,+\infty)$. For every $\Psi \in L_2(\Omega)$ and all $j \geqslant 0$ we denote $U_j := (-\Delta^{\mathbb{R}}+\mu_j^2-z)^{-1}\Psi_j \in L^2(\mathbb{R})$, where Ψ_j are defined in Lemma 11.3. It is clear that

$$\|U_j\|_{L_2(\mathbb{R})} \leqslant \frac{\|\Psi_j\|_{L_2(\mathbb{R})}}{\operatorname{dist}\big(z,[\mu_j^2,+\infty)\big)} \leqslant C\,\frac{\|\Psi_j\|_{L_2(\mathbb{R})}}{j^2+1}\,, \quad \|U_j'\|_{L_2(\mathbb{R})} \leqslant C\,\frac{\|\Psi_j\|_{L_2(\mathbb{R})}}{\sqrt{j^2+1}}\,, \tag{11.28}$$

where C is a constant depending uniquely on $|\alpha_0|$, d and z; the second inequality follows from the identity $\|U_j'\|^2_{L_2(\mathbb{R})}+(\mu_j^2-z)\|U_j\|^2_{L_2(\mathbb{R})} = (\Psi_j,U_j)_{L_2(\mathbb{R})}$. Using (11.28) and estimates of the type (11.27), it is readily seen that each function $R_j : x \mapsto U_j(x_1)\psi_j(x_2)$ belongs to $W_2^1(\Omega)$. We will show that it is the case for their infinite sum too. Firstly, a consecutive use of (11.25), the first inequality of (11.28) and (11.26) together with Fubini's theorem implies $\|\sum_{j=2}^n R_j\|_{L_2(\Omega)} \leqslant K\,\|\Psi\|_{L_2(\Omega)}$, where K is a constant independent of $n \geqslant 2$. Secondly, a similar estimate for the partial sum of $\partial_1 R_j$ can be obtained in the same way, provided that one uses the second inequality of (11.28) now. Finally, since the derivative of ψ_j as well can be expressed in terms of χ_j^N and χ_j^D introduced in the proof of Lemma 11.3, a consecutive use of the estimates of the type (11.25) and the first inequality of (11.28) together with Fubini's theorem implies

$$\Big\|\sum_{j=2}^n \partial_2 R_j\Big\|^2_{L_2(\Omega)} \leqslant d\sum_{j=2}^n(\alpha_0^2+\mu_j^2)\|U_j\|^2_{L_2(\mathbb{R})} \leqslant d\,C^2\sum_{j=2}^n\frac{\alpha_0^2+\mu_j^2}{(j^2+1)^2}\|\Psi_j\|^2_{L_2(\mathbb{R})}\,;$$

here the fraction in the upper bound forms a bounded sequence in j, so that we may continue to estimate as above using (11.26) together with Fubini's theorem again. Summing up, the series $\sum_{j=0}^\infty R_j$ converges in $W_2^1(\Omega)$ to a function R and

$$\|R\|_{W_2^1(\Omega)} \leqslant \tilde{K}\,\|\Psi\|_{L_2(\Omega)}\,,$$

where $\tilde{K}$ depends uniquely on $|\alpha_0|$, d and z. Employing this fact and the definition of U_j, one can check easily that R satisfies the identity $h_{\alpha_0}(R,\Phi)-z(R,\Phi)_{L_2(\Omega)} = (\Psi,\Phi)_{L_2(\Omega)}$ for all $\Phi \in W_2^1(\Omega)$. It implies that $R \in \mathfrak{D}(H_{\alpha_0})$ and $(H_{\alpha_0}-z)R = \Psi$, i.e., $R = (H_{\alpha_0}-z)^{-1}\Psi$. □

Lemmata 11.4 and 11.5 yield

Proposition 11.5. *Let* $\alpha_0 \in \mathbb{R}$*. Then*

$$\sigma_{\mathrm{e}}(H_{\alpha_0}) = [\mu_0^2,+\infty)\,.$$

Proof. In view of the lemmata, the result holds for every $\alpha_0 \in \mathbb{R}$ except for a discrete set of points complementary to the hypothesis (11.14). However, these points can be included by noticing that $\alpha_0 \mapsto H_{\alpha_0}$ forms a holomorphic family of operators (*cf* Remark 11.3). □

Proposition 11.5 and Proposition 11.4 together with Remark 11.3 imply that the spectrum of H_{α_0} is real and (11.10) holds true for every $\alpha_0 \in \mathbb{R}$.

Remark 11.4. It follows from (11.10) that the spectrum of H_{α_0} is equal to the sum of the spectra of $-\Delta^{\mathbb{R}}$ and $-\Delta^{I}_{\alpha_0}$. This result could alternatively be obtained by using a general theorem about the spectrum of tensor products [25, Thm. XIII.35] and the fact that the one-dimensional operators generate bounded holomorphic semigroups. However, we do not use this way of proof since Lemma 11.5 is employed not only in the proof of (11.10) but also in the proofs of Theorems 11.5 and 11.6.

11.5 Stability of the essential spectrum

In this section we show that the essential spectrum is stable under a compactly supported perturbation of the boundary conditions. In fact, we will establish a stronger result, namely that the difference of the resolvents of H_α and H_{α_0} is a compact operator. As an auxiliary result, we shall need the following lemma.

Lemma 11.6. *Let $\alpha_0 \in \mathbb{R}$ and $\varphi \in L^2(\partial\Omega)$. There exist positive constants c and C, depending on d and $|\alpha_0|$, such that any solution $\Psi \in W_2^1(\Omega)$ of the boundary value problem*

$$\begin{cases} (-\Delta - z)\Psi = 0 & \text{in} \quad \Omega\,, \\ (\partial_2 + \mathrm{i}\alpha_0)\Psi = \varphi & \text{on} \quad \partial\Omega\,, \end{cases} \tag{11.29}$$

with any $z \leqslant -c$, satisfies the estimate

$$\|\Psi\|_{W_2^1(\Omega)} \;\leqslant\; C\,\|\varphi\|_{L^2(\partial\Omega)}\,. \tag{11.30}$$

Proof. Multiplying the first equation of (11.29) by $\overline{\Psi}$ and integrating over Ω, we arrive at the identity

$$\|\nabla\Psi\|^2 - z\,\|\Psi\|^2 + \mathrm{i}\alpha_0 \int_{\partial\Omega} \nu_2\,|\Psi|^2 - \int_{\partial\Omega} \nu_2\,\varphi\overline{\Psi} = 0\,, \tag{11.31}$$

where ν_2 denotes the second component of the outward unit normal vector to $\partial\Omega$. Using the Schwarz and Cauchy inequalities together with $|\nu_2| = 1$, we have

$$\begin{aligned} \left|\int_{\partial\Omega} \nu_2\,|\Psi|^2\right| &= \left|\int_{\Omega} \partial_2|\Psi|^2\right| = 2\,|\mathrm{Re}\,(\Psi, \partial_2\Psi)| \leqslant \delta^{-1}\,\|\Psi\|^2 + \delta\,\|\nabla\Psi\|^2\,, \\ 2\left|\int_{\partial\Omega} \nu_2\,\varphi\overline{\Psi}\right| &\leqslant \delta^{-1}\,\|\varphi\|_{L^2(\partial\Omega)} + \delta\,\|\Psi\|_{L^2(\partial\Omega)}\,, \end{aligned}$$

with any $\delta \in (0,1)$. Here $\|\Psi\|_{L^2(\partial\Omega)} \leqslant C\,\|\Psi\|_{W_2^1(\Omega)}$, where C is the constant coming from the embedding of $W_2^1(\Omega)$ in $L^2(\partial\Omega)$ (depending only on d in our case). Choosing now sufficiently small δ and sufficiently large negative z, it is clear that (11.31) can be cast into the inequality (11.30). □

Now we are in a position to prove

Proposition 11.6. *Let $\alpha - \alpha_0 \in C_0(\mathbb{R}) \cap W^1_\infty(\mathbb{R})$ with $\alpha_0 \in \mathbb{R}$. Then*

$$(H_\alpha - z)^{-1} - (H_{\alpha_0} - z)^{-1} \quad \textit{is compact in } L^2(\Omega)$$

for any $z \in \rho(H_\alpha) \cap \rho(H_{\alpha_0})$.

Proof. It is enough to prove the result for one z in the intersection of the resolvent sets of H_α and H_{α_0}, and we can assume that the one is negative (since the operators are m-accretive). Given $\Phi \in L^2(\Omega)$, let $\Psi := (H_\alpha - z)^{-1}\Phi - (H_{\alpha_0} - z)^{-1}\Phi$. It is easy to check that Ψ is the unique solution to (11.29) with $\varphi := -\mathrm{i}(\alpha - \alpha_0)T(H_\alpha - z)^{-1}\Phi$, where T denotes the trace operator from $W_2^2(\Omega) \supset \mathsf{D}(H_\alpha)$ to $W_2^1(\partial\Omega)$. By virtue of Lemma 11.6, it is therefore enough to show that $(\alpha - \alpha_0)T(H_\alpha - z)^{-1}$ is a compact operator from $L^2(\Omega)$ to $L^2(\partial\Omega)$. However, this property follows from the fact that $W_2^1(\partial\Omega)$ is compactly embedded in $L^2(\omega)$ for every bounded subset ω of $\partial\Omega$, due to the Rellich-Kondrachov theorem [1, Sec. VI]. □

Corollary 11.2. *Suppose the hypothesis of Proposition 11.6. Then*

$$\sigma_{\mathrm{e}}(H_\alpha) = [\mu_0^2, +\infty)\,.$$

Proof. Our definition of essential spectrum is indeed stable under relatively compact perturbations [11, Thm. IX.2.4]. □

11.6 Point spectrum

In this section we prove Theorems 11.3–11.6 and Propositions 11.1–11.2. In the proofs of Theorems 11.4–11.6 we follow the main ideas of [13]. Throughout this section we assume that the identity (11.16) and the assumption (11.14) hold true.

11.6.1 Proof of Theorem 11.3

Any eigenvalue of infinite geometric multiplicity belongs to the essential spectrum which is real by Theorem 11.2. Let λ be an eigenvalue of H_α of finite geometric multiplicity, and Ψ be an associated eigenfunction. Using that α is of compact support, it is easy to check that $x \mapsto \Psi(-x_1, d-x_2)$ is an eigenfunction associated with λ, too. The geometric multiplicity of λ being finite, we conclude that at least one of the eigenfunction associated with λ satisfies $|\Psi(x)| = |\Psi(-x_1, d-x_2)|$. Taking this identity into account, integrating by parts and using the hypothesis that α is odd, we obtain

$$\lambda \, \|\Psi\|^2_{L_2(\Omega)} = h^1_\alpha[\Psi] + \mathrm{i} h^2_\alpha[\Psi] = \|\nabla\Psi\|^2_{L_2(\Omega)} \, ,$$

which implies that λ is real. □

11.6.2 Auxiliary results

Let a function $F \in L_2(\Omega)$ be such that $\operatorname{supp} F \subseteq \overline{\Omega_b}$ for fixed $b > 0$. We consider the boundary value problem

$$\begin{cases} -\Delta U = (\mu_0^2 - k^2)U + F & \text{in} \quad \Omega \, , \\ (\partial_2 + \mathrm{i}\alpha_0)\, U = 0 & \text{on} \quad \partial\Omega \, , \end{cases} \tag{11.32}$$

where the parameter $k \in \mathbb{C}$ ranges in a small neighbourhood of zero. The problem can be solved by separation of variables justified in Lemma 11.5 whenever $k^2 \notin (-\infty, 0]$. Moreover, it is possible to extend the solution of (11.32) analytically with respect to k. Namely, the following statement is valid.

Lemma 11.7. *For all small $k \in \mathbb{C}$ there exists the unique solution to* (11.32) *satisfying*

$$U(x;k) = c_\pm(k) \mathrm{e}^{-k|x_1|}\psi_0(x_2) + \mathcal{O}\big(\mathrm{e}^{-\operatorname{Re}\sqrt{\mu_1^2-\mu_0^2+k^2}|x_1|}\big) \, , \tag{11.33}$$

in the limit $x_1 \to \pm\infty$, where $c_\pm(k)$ are constants. The mapping $T_1(k)$ defined as $T_1(k)F := U$ is a bounded linear operator from $L_2(\Omega_b)$ into $W_2^2(\Omega_a)$ for each $a > 0$. This operator is meromorphic with respect to k and has the simple pole at zero,

$$T_1(k)F = \frac{\psi_0}{2k} \int\limits_\Omega F(x)\overline{\phi_0}(x_2)\, \mathrm{d}x + T_2(k)F,$$

where for each $a > 0$ the operator $T_2(k) : L_2(\Omega_b) \to W_2^2(\Omega_a)$ is linear, bounded and holomorphic with respect to k small enough. The function $\widehat{U} := T_2(0)F$ is the unique solution to the problem

$$\begin{cases} -\Delta \widehat{U} = \mu_0^2 \widehat{U} + F \quad \text{in} \quad \Omega, \qquad (\partial_2 + \mathrm{i}\alpha_0)\, \widehat{U} = 0 \quad \text{on} \quad \partial\Omega, \\ \widehat{U}(x) = -\dfrac{\psi_0(x_2)}{2} \displaystyle\int\limits_\Omega |x_1 - t_1| F(t)\overline{\phi_0}(t_2)\, \mathrm{d}t + \mathcal{O}\big(\mathrm{e}^{-\sqrt{\mu_1^2-\mu_0^2}|x_1|}\big), \quad |x_1| \to +\infty, \end{cases} \tag{11.34}$$

given by the formula

$$\widehat{U}(x) = \sum_{j=0}^{\infty} \widehat{U}_j(x_1)\psi_j(x_2) \tag{11.35}$$

with

$$\widehat{U}_j(x_1) := \begin{cases} -\dfrac{1}{2} \displaystyle\int\limits_\Omega |x_1 - t_1| F(t)\overline{\phi_0}(t_2)\, \mathrm{d}t & \text{if} \quad j = 0 \, , \\ \dfrac{1}{2\sqrt{\mu_j^2 - \mu_0^2}} \displaystyle\int\limits_\Omega \mathrm{e}^{-\sqrt{\mu_j^2-\mu_0^2}|x_1-t_1|} F(t)\overline{\phi_j}(t_2)\, \mathrm{d}t & \text{if} \quad j \geqslant 1 \, . \end{cases}$$

The lemma is proved in the same way as Lemma 3.1 in [4].

Let M_ε be the operator of multiplication by the function $x \mapsto \mathrm{e}^{-\mathrm{i}\varepsilon\beta(x_1)x_2}$. It is straightforward to check that H_α is unitarily equivalent to the operator

$$M_\varepsilon^{-1} H_\alpha M_\varepsilon = H_{\alpha_0} - \varepsilon L_\varepsilon\,,$$

where

$$L_\varepsilon = -2\mathrm{i}\beta'(x_1)x_2\frac{\partial}{\partial x_1} - 2\mathrm{i}\beta(x_1)\frac{\partial}{\partial x_2} - \big(\varepsilon\beta^2(x_1) + \mathrm{i}\beta''(x_1)x_2 + \varepsilon\beta'^2(x_1)x_2^2\big)\,.$$

We observe that the coefficients of L_ε are compactly supported and that their supports are bounded uniformly in ε.

It follows that the eigenvalue equation for H_α is equivalent to

$$H_{\alpha_0}U = \lambda U + \varepsilon L_\varepsilon U,$$

where an eigenfunction Ψ of H_α satisfies $\Psi = M_\varepsilon U$. It can be rewritten as

$$\begin{cases} \quad -\Delta U = (\mu_0^2 - k^2)U + \varepsilon L_\varepsilon U & \text{in} \quad \Omega\,, \\ (\partial_2 + \mathrm{i}\alpha_0)U = 0 & \text{on} \quad \partial\Omega\,, \end{cases} \tag{11.36}$$

where we have replaced λ by $\mu_0^2 - k^2$.

Now, let λ be an eigenvalue for H_α close to μ_0^2. As $x_1 \to \pm\infty$, the solution U to (11.36) satisfies the asymptotic formula (11.33), where $k = \sqrt{\mu_0^2 - \lambda}$ and the branch of the root is specified by the requirement $\operatorname{Re} k > 0$. Such restriction guarantees that the function U together with their derivatives decays exponentially at infinity and thus belongs to $W_2^2(\Omega)$. Hence, the set of all k for which the problem (11.36), (11.33) has a nontrivial solution includes the set of all values of k related to the eigenvalues of H_α by the relation $\lambda = \mu_0^2 - k^2$. Thus, it is sufficient to find all small k for which a nontrivial solution to (11.36), (11.33) exists and to check whether the solution belongs to $W_2^2(\Omega)$. If it does, the corresponding number $\lambda = \mu_0^2 - k^2$ is an eigenvalue of H_α.

We introduce the numbers

$$k_1(\varepsilon) := \frac{1}{2}\int\limits_\Omega \overline{\phi_0}(x_2)(L_\varepsilon\psi_0)(x)\,\mathrm{d}x\,, \quad k_2(\varepsilon) := \frac{1}{2}\int\limits_\Omega \overline{\phi_0}(x_2)\big(L_\varepsilon T_2(0)L_\varepsilon\psi_0\big)(x)\,\mathrm{d}x\,.$$

Basing on Lemma 11.7 and arguing in the same way as in [13, Sec. 2] one can prove easily the following statement (see also [4, Sec. 4]).

Lemma 11.8. *There exists the unique function $\varepsilon \mapsto k(\varepsilon)$ converging to zero as $\varepsilon \to +0$ for which the problem* (11.36)*,* (11.33) *has a nontrivial solution. It satisfies the asymptotics*

$$k(\varepsilon) = \varepsilon k_1(\varepsilon) + \varepsilon^2 k_2(\varepsilon) + \mathcal{O}(\varepsilon^3).$$

The associated nontrivial solution to (11.36)*,* (11.33) *is unique up to a multiplicative constant and can be chosen so that it obeys* (11.33) *with*

$$c_\pm(k(\varepsilon)) = 1 + \mathcal{O}(\varepsilon), \quad \varepsilon \to +0, \tag{11.37}$$

as well as

$$U(x;\varepsilon) = \psi_0(x_2) + \mathcal{O}(\varepsilon)$$

in $W_2^2(\Omega_a)$ for each fixed $a > 0$.

11.6.3 Proof of Theorems 11.5 and 11.6

It follows from Lemma 11.8 that there is at most one simple eigenvalue of H_α converging to μ_0^2 as $\varepsilon \to +0$. A sufficient condition guaranteeing the existence of such eigenvalue is the inequality

$$\operatorname{Re}\big(k_1(\varepsilon) + \varepsilon k_2(\varepsilon)\big) \geqslant C(\varepsilon)\,\varepsilon^2, \qquad C(\varepsilon) \to +\infty, \quad \varepsilon \to +0, \tag{11.38}$$

that is implied by (11.33), (11.37), the definition of the operator M_ε and the assumption on β. The sufficient condition of the absence of the eigenvalue is the opposite inequality

$$\operatorname{Re}\big(k_1(\varepsilon) + \varepsilon k_2(\varepsilon)\big) \leqslant -C(\varepsilon)\,\varepsilon^2, \qquad C(\varepsilon) \to +\infty, \quad \varepsilon \to +0. \tag{11.39}$$

Thus, we just need to calculate the numbers k_1 and k_2 to prove the theorems.

It is easy to compute the coefficient k_1,

$$k_1(\varepsilon) = \begin{cases} -\alpha_0\langle\beta\rangle + k_1'(0)\,\varepsilon & \text{if} \quad |\alpha_0| < \pi/d\,, \\ k_1'(0)\,\varepsilon & \text{if} \quad |\alpha_0| > \pi/d\,, \end{cases} \tag{11.40}$$

where

$$k_1'(0) := -\frac{1}{2}\int\limits_{\Omega} \psi_0(x_2)\overline{\phi_0}(x_2)\big(\beta^2(x_1) + \beta'^2(x_1)\,x_2^2\big)\,\mathrm{d}x\,.$$

It is more complicated technically to calculate k_2. This coefficient depends on ε as well; to prove the theorem we need the leading term of its asymptotics as $\varepsilon \to +0$. We begin the calculations by observing an obvious identity,

$$L_\varepsilon U = L_0 U + \mathcal{O}(\varepsilon)\,,$$

where

$$\begin{aligned}(L_0U)(x) :=& -2\mathrm{i}\beta'(x_1)x_2\frac{\partial U(x)}{\partial x_1} - 2\mathrm{i}\beta(x_1)\frac{\partial U(x)}{\partial x_2} - \mathrm{i}\beta''(x_1)x_2U(x) \\ =&\, \mathrm{i}\Big(\beta(x_1)x_2\Delta U(x) - \Delta\big[\beta(x_1)x_2U(x)\big]\Big),\end{aligned}$$

which is valid for each $U \in W^2_{2,loc}(\Omega)$ in $L_2(\Omega_a)$, if a is large enough and independent of ε. Thus,

$$k_2(\varepsilon) = k_2(0) + \mathcal{O}(\varepsilon), \qquad \text{where} \qquad k_2(0) = \frac{1}{2}\int\limits_{\Omega} \overline{\phi_0}(x_2)\big(L_0T_2(0)L_0\psi_0\big)(x)\,\mathrm{d}x.$$

We denote $\widehat{U} := T_2(0)\widehat{F}$ and $\widehat{F} := L_0\psi_0$. Taking into account the problem (11.34) for $\widehat{U}$ and integrating by parts, we obtain

$$\begin{aligned} k_2(0) =& \frac{\mathrm{i}}{2}\int\limits_{\Omega} \overline{\phi_0}(x_2)\,\Big(\beta(x_1)x_2\Delta\widehat{U}(x) - \Delta\big[\beta(x_1)x_2\widehat{U}(x)\big]\Big)\,\mathrm{d}x \\ =& -\frac{\mathrm{i}}{2}\int\limits_{\Omega} \overline{\phi_0}(x_2)(\Delta + \mu_0^2)\beta(x_1)x_2\widehat{U}(x)\,\mathrm{d}x - \frac{\mathrm{i}}{2}\int\limits_{\Omega} \overline{\phi_0}(x_2)\beta(x_1)x_2\widehat{F}(x)\,\mathrm{d}x \\ =& -\frac{\mathrm{i}}{2}\left\langle\beta\left[\overline{\phi_0}(d)\widehat{U}(\cdot,d) - \overline{\phi_0}(0)\widehat{U}(\cdot,0)\right]\right\rangle - \frac{\mathrm{i}}{2}\int\limits_{\Omega} \overline{\phi_0}(x_2)\beta(x_1)x_2\widehat{F}(x)\,\mathrm{d}x\,. \end{aligned} \tag{11.41}$$

The last term on the right hand side of this identity is calculated by integration by parts,

$$\begin{aligned} -\frac{\mathrm{i}}{2}&\int\limits_{\Omega} \overline{\phi_0}(x_2)\beta(x_1)x_2\widehat{F}(x)\,\mathrm{d}x \\ &= -\frac{1}{2}\int\limits_{\Omega} \overline{\phi_0}(x_2)\beta(x_1)x_2\big[2\beta(x_1)\psi_0'(x_2) + \beta''(x_1)x_2\psi_0(x_2)\big]\,\mathrm{d}x \\ &= -\frac{1}{2}\int\limits_{\Omega} \beta^2(x_1)x_2\left(\overline{\phi_0}\psi_0\right)'(x_2)\,\mathrm{d}x + \frac{1}{2}\int\limits_{\Omega} x_2^2\beta'^2(x_1)\overline{\phi_0}(x_2)\psi_0(x_2)\,\mathrm{d}x \\ &= -\frac{\overline{\phi_0}(d)\psi_0(d)d}{2}\langle\beta^2\rangle + \frac{1}{2}\int\limits_{\Omega} \overline{\phi_0}(x_2)\psi_0(x_2)\big[\beta^2(x_1) + \beta'^2(x_1)x_2^2\big]\,\mathrm{d}x\,. \end{aligned}$$

This formula, (11.40) and (11.41) yield

$$k_1(\varepsilon) + \varepsilon k_2(\varepsilon) = \begin{cases} -\varepsilon\alpha_0\langle\beta\rangle + \varepsilon^2 K + \mathcal{O}(\varepsilon^3) & \text{if} \quad |\alpha_0| < \pi/d\,, \\ \varepsilon^2 K + \mathcal{O}(\varepsilon^3) & \text{if} \quad |\alpha_0| > \pi/d\,, \end{cases} \tag{11.42}$$

where

$$K := -\frac{\mathrm{i}}{2}\left\langle\beta\left[\overline{\phi_0}(d)\widehat{U}(\cdot,d) - \overline{\phi_0}(0)\widehat{U}(\cdot,0)\right]\right\rangle - \frac{\overline{\phi_0}(d)\psi_0(d)d}{2}\langle\beta^2\rangle.$$

Thus, it remains to calculate K. In order to do it, we construct the function $\widehat{U}$ as the series (11.35).

Case $\underline{|\alpha_0| < \pi/d}$**:** Using the identity

$$\widehat{F}(x) = -2\mathrm{i}\beta(x_1)\psi_0'(x_2) - \mathrm{i}\beta''(x_1)x_2\psi_0(x_2)\,,$$

one can check that

$$\widehat{F}(x) = -2\alpha_0\beta(x_1)\psi_0(x_2) - \mathrm{i}\beta''(x_1)\sum_{j=0}^{\infty} c_j\psi_j(x_2)\,,$$

$$\widehat{U}_j(x_1) = \begin{cases} \mathrm{i}c_0\beta(x_1) - 2\alpha_0 v_0(x_1) & \text{if} \quad j=0\,,\\ \mathrm{i}c_j\big[\beta(x_1) - (\mu_j^2-\mu_0^2)v_j(x_1)\big] & \text{if} \quad j\geqslant 1\,,\end{cases}$$

where $c_j := \int_I x_2\psi_0(x_2)\overline{\phi_j}(x_2)dx_2$ and the functions v_j were introduced in (11.17). Substituting now the formulae for $\widehat{U}_j$ and (11.35) into (11.42), we arrive at the following chain of identities

$$\begin{aligned} K =& \frac{1}{2}\Big[\sum_{j=0}^{\infty} c_j\psi_j(x_2)\overline{\phi}_0(x_2)\Big]_{x_2=0}^{x_2=d}\langle\beta^2\rangle + 2\alpha_0^2\langle\beta v_0\rangle \\ &- \frac{2\alpha_0}{d}\sum_{j=1}^{\infty}\frac{\mathrm{i}\big[\mathrm{e}^{\mathrm{i}\alpha_0 d} - (-1)^j\big]\mu_j^2}{\big[\mathrm{e}^{\mathrm{i}\alpha_0 d} + (-1)^j\big](\mu_j^2-\mu_0^2)}\langle\beta v_j\rangle - \frac{\overline{\phi}_0(d)\psi_0(d)d}{2}\langle\beta^2\rangle \\ =& \frac{1}{2}\Big[x_2\psi_0(x_2)\overline{\phi}_0(x_2)\Big]_{x_2=0}^{x_2=d}\langle\beta^2\rangle + 2\alpha_0^2\langle\beta v_0\rangle \\ &+ \frac{2\alpha_0}{d}\sum_{j=1}^{\infty}\frac{\mu_j^2\langle\beta v_j\rangle}{\mu_j^2-\mu_0^2}\tan\frac{\alpha_0 d+\pi j}{2} - \frac{\overline{\phi}_0(d)\psi_0(d)d}{2}\langle\beta^2\rangle\,, \end{aligned}$$

where the last expression coincides with τ for $|\alpha_0| < \pi/d$.

Case $\underline{|\alpha_0| > \pi/d}$**:** Following the same scheme as above, we arrive at

$$\begin{aligned} \widehat{F}(x) =& -\mathrm{i}\beta''(x_1)\sum_{j=0}^{\infty} c_j\psi_j(x_2) - \frac{4\alpha_0\psi_1(x_2)\beta(x_1)}{1-\mathrm{e}^{-\mathrm{i}\alpha_0 d}} \\ &- \frac{2\mathrm{i}}{d}(\mu_0^2-\mu_1^2)\sum_{j=1}^{\infty}\frac{\mu_{2j}^2\psi_{2j}(x_2)}{(\mu_{2j}^2-\mu_1^2)(\mu_{2j}^2-\mu_0^2)}\beta(x_1)\,, \end{aligned}$$

$$\widehat{U}_j(x_1) = \begin{cases} \mathrm{i}c_0\beta(x_1) & \text{if} \quad j=0\,,\\ \mathrm{i}c_1\beta(x_1) - \dfrac{2\alpha_0}{1-\mathrm{e}^{-\mathrm{i}\alpha_0 d}}v_1(x_1) & \text{if} \quad j=1\,,\\ \mathrm{i}c_j\beta(x_1) + \dfrac{2\mathrm{i}\mu_j^2\big[1+(-1)^j\big]}{(\mu_j^2-\mu_1^2)d}v_j(x_j) & \text{if} \quad j\geqslant 2\,,\end{cases}$$

and check that $K=\tau$ for $|\alpha_0| > \pi/d$.

The series in the formulae for τ converge since the functions v_j satisfy

$$-v_j'' + (\mu_j^2-\mu_0^2)v_j = \beta \qquad \text{in} \quad \mathbb{R}\,, \tag{11.43}$$

and by [18, Ch. V, §3.5, Formula (3.16)] ($j\geqslant 1$)

$$|\langle\beta v_j\rangle| \leqslant \|\beta\|_{L_2(\mathbb{R})}\|v\|_{L_2(\mathbb{R})} \leqslant \frac{\|\beta\|_{L_2(\mathbb{R})}^2}{\mu_j^2-\mu_0^2}. \tag{11.44}$$

Summing up,

$$k_1(\varepsilon) + \varepsilon k_2(\varepsilon) = \begin{cases} -\varepsilon\alpha_0\langle\beta\rangle + \varepsilon^2\tau + \mathcal{O}(\varepsilon^3) & \text{if} \quad |\alpha_0| < \pi/d\,,\\ \varepsilon^2\tau + \mathcal{O}(\varepsilon^3) & \text{if} \quad |\alpha_0| > \pi/d\,.\end{cases}$$

All the statements of the theorems – except for the reality of the eigenvalue – follow from these formulae, the identity $\lambda = \mu_0^2 - k^2$, the inequalities (11.38) and (11.39), Lemma 11.8, the asymptotics (11.33) for U, and the definition of the operator M_ε.

Let us show that λ_ε is necessarily real as $\varepsilon\to 0+$. Let Ψ_ε be the eigenfunction associated with the eigenvalue λ_ε. It is easy to check that the function $x\mapsto\overline{\Psi}_\varepsilon(x_1, d-x_2)$ is an eigenfunction of H_α associated with the eigenvalue $\overline{\lambda}_\varepsilon$. This eigenvalue converges to μ_0^2 as $\varepsilon\to +0$. By the uniqueness of such eigenvalue we obtain $\lambda_\varepsilon = \overline{\lambda}_\varepsilon$ that completes the proof. ∎

11.6.4 Proof of Theorem 11.4

We employ here the same argument as in the previous proof. The formula for $k(\varepsilon)$ in the case $\alpha_0 = 0$ can be obtained from that for $|\alpha_0| < \pi/d$ by passing to the limit $\alpha_0 \to 0$. It leads us to the relation

$$k(\varepsilon) = \varepsilon^2\tau + \mathcal{O}(\varepsilon^3) \qquad \text{with} \qquad \tau = -\sum_{j=0}^{\infty} \frac{4\langle \beta v_{2j+1}\rangle}{\mu_{2j+1} d^2}\,.$$

To prove the theorem it is sufficient to show that $\tau < 0$. Indeed, the equation (11.43) implies that for $j \geqslant 1$

$$\langle \beta v_j\rangle = \|v_j'\|^2_{L_2(\mathbb{R})} + (\mu_j^2 - \mu_0^2)\|v_j\|^2_{L_2(\mathbb{R})} > 0\,. \tag{11.45}$$

Thus, $\tau < 0$. ☐

11.6.5 Proof of Proposition 11.1

Since $\langle\beta\rangle = 0$, the function v_0 is constant at infinity. Hence, by the equation (11.43) for v_0,

$$\langle \beta v_0\rangle = \|v_0'\|^2_{L_2(\mathbb{R})}.$$

At the same time, it follows from (11.44) and (11.45) that for $j \geqslant 1$,

$$0 < \langle \beta v_j\rangle < \frac{\|\beta\|^2_{L_2(\mathbb{R})}}{\mu_j^2 - \mu_0^2}.$$

The relations obtained allow us to estimate

$$\begin{aligned}
\tau &> 2\alpha_0^2\|v_0'\|^2_{L_2(\mathbb{R})} - \frac{2\alpha_0 \cot\frac{\alpha_0 d}{2}}{d}\|\beta\|^2_{L_2(\mathbb{R})}\left(\frac{\mu_1^2}{(\mu_1^2-\mu_0^2)^2} + \sum_{j=1}^{\infty}\frac{\mu_{2j+1}^2}{(\mu_{2j+1}^2 - \mu_1^2)^2}\right)\\
&= \frac{\alpha_0^2 l^3}{2}\left\|\int_{\mathbb{R}} \operatorname{sgn}(\cdot - t_1)\widetilde{\beta}(t_1)\,\mathrm{d}t_1\right\|^2_{L_2(\mathbb{R})}\\
&\quad - \frac{2\alpha_0 l \cot\frac{\alpha_0 d}{2}}{d}\left(\frac{\mu_1^2}{(\mu_1^2-\mu_0^2)^2} + \frac{d^2}{16\pi^2} + \frac{d^2}{48}\right)\|\widetilde{\beta}\|^2_{L_2(\mathbb{R})}\,,
\end{aligned}$$

where the resulting expression is positive under the hypothesis. ☐

11.6.6 Proof of Proposition 11.2

Using (11.45), we obtain

$$\tau > \frac{2\alpha_0\pi^2\cot\frac{\alpha_0 d}{2}}{(\mu_1^2-\mu_0^2)d^3}\langle\beta v_1\rangle + \frac{8\pi^2}{(\mu_1^2-\mu_0^2)d^4}\sum_{j=1}^{m}\frac{\mu_{2j}^2\langle\beta v_{2j}\rangle}{\mu_{2j}^2-\mu_1^2}\,,$$

where the right hand side is non-negative under the hypothesis (11.21). ☐

Let us show that the inequality (11.21) can be achieved if $\alpha_0 \to \mu_2 + 0$. In this case $m = 1$, and it is sufficient to check that

$$\alpha_0\langle\beta v_1\rangle\cot\frac{\alpha_0 d}{2} > \frac{16\pi^2\langle\beta v_2\rangle}{(\mu_1^2-\mu_2^2)d^3} = \frac{16\pi^2\langle\beta v_2\rangle}{(\alpha_0^2-\mu_2^2)d^3}. \tag{11.46}$$

It follows from the definition of v_1 that it satisfies the asymptotic formula

$$v_1(x_1) = v_2(x_1) + (\mu_2 - \alpha_0)\,\widehat{v}(x_1) + \mathcal{O}\big((\mu_2-\alpha_0)^2\big)$$

in $L_2(\mathbb{R})$-norm, where the function $\widehat{v}$ is given by

$$\widehat{v}(x_1) := \int_{\mathbb{R}} \frac{(\sqrt{3}\mu_0|x_1-t_1|+1)\mathrm{e}^{-\sqrt{3}\mu_0|x_1-t_1|}}{3\sqrt{3}\mu_0^2}\beta(t_1)\,\mathrm{d}t_1,$$

and satisfies the equation

$$-\widehat{v}'' + 3\mu_0^2\,\widehat{v} = 4\mu_0 v_2 \qquad \text{in} \quad \mathbb{R}.$$

We multiply this equation by v_2 and integrate by parts over $\mathbb{R}$ taking into account the equation (11.43) for v_2,

$$4\mu_0\|v_2\|^2_{L_2(\mathbb{R})} = \langle\beta\widehat{v}\rangle.$$

Hence,

$$\langle\beta v_1\rangle = \langle\beta v_2\rangle + 4(\mu_2-\alpha_0)\mu_0\|v_2\|^2_{L_2(\mathbb{R})} + \mathcal{O}\big((\mu_2-\alpha_0)^2\big).$$

Employing this identity, we write the asymptotic expansions for the both sides of (11.46) as $\alpha_0 \to \mu_2+0$, and obtain

$$\begin{aligned}\alpha_0\langle\beta v_1\rangle\cot\frac{\alpha_0 d}{2} &= \frac{4\pi\langle\beta v_2\rangle}{(\alpha_0-\mu_2)d^2} + \frac{2}{d}\left(\langle\beta v_2\rangle - \frac{8\pi^2}{d^2}\|v_2\|^2_{L_2(\mathbb{R})}\right) + \mathcal{O}(\mu_2-\alpha_0)\,,\\ \frac{16\pi^2\langle\beta v_2\rangle}{(\alpha_0^2-\mu_2^2)d^3} &= \frac{4\pi\langle\beta v_2\rangle}{(\alpha_0-\mu_2)d^2} - \frac{\langle\beta v_2\rangle}{d} + \mathcal{O}(\mu_2-\alpha_0)\,.\end{aligned}$$

Thus, to satisfy (11.46), it is sufficient to check that

$$3\langle\beta v_2\rangle - \frac{16\pi^2}{d^2}\|v_2\|^2_{L_2(\mathbb{R})} > 0\,,$$

which is in view of (11.45) equivalent to

$$3\|v_2'\|^2_{L_2(\mathbb{R})} > \frac{7\pi^2}{d^2}\|v_2\|^2_{L_2(\mathbb{R})}\,.$$

It is clear that there exists a function $v \in C_0^\infty(\mathbb{R})$ for which this inequality is valid. Letting $v_2 := v$ and $\beta := -v'' + 3\mu_0^2 v$, we conclude that there exists β such that the inequality (11.21) holds true, if α_0 is sufficiently close to μ_2 and greater than this number.

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Erratum

1. There is a mistake in the proof of Theorem 11.3 given in Section 11.6.1. At this moment, we do not know whether Theorem 11.3 holds.

Chapter 12

Non-Hermitian spectral effects in a $\mathcal{PT}$-symmetric waveguide

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Non-Hermitian spectral effects in a $\mathcal{PT}$-symmetric waveguide

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Abstract. We present a numerical study of the spectrum of the Laplacian in an unbounded strip with $\mathcal{PT}$-symmetric boundary conditions. We focus on non-Hermitian features of the model reflected in an unusual dependence of the eigenvalues below the continuous spectrum on various boundary-coupling parameters.

12.1 Introduction

In the last years the theory of quasi-Hermitian, pseudo-Hermitian and $\mathcal{PT}$-symmetric operators has developed rapidly, and has been shown to provide a huge class of non-Hermitian Hamiltonians with real spectra (*cf* the pioneering works [24, 4, 23] and the review [3] with many references). Because of these recent observations, the condition of self-adjointness of operators representing observables in quantum mechanics may seem to be rather an annoying technicality. However, unless it is met one cannot apply the very powerful machinery of spectral theory based on the spectral theorem.

In particular, one has to restrict to exactly solvable models [22, 27, 25, 18, 21] or to rely on perturbation and numerical methods to analyse the spectrum of the $\mathcal{PT}$-symmetric Hamiltonians. Except for some simple one-dimensional examples [2], the majority of the $\mathcal{PT}$-symmetric models studied in the literature have purely discrete spectrum. Perturbation methods are then notably effective in determining the dependence of the eigenvalues on various parameters of the given model. Although the perturbation approach can even prove that the total spectrum is real in some cases [20, 8, 7, 9], it is limited in its nature and one usually has to employ numerical techniques in order to obtain a more complete picture of the spectral properties.

In a way motivated by the lack of a well-developed spectral theory for non-self-adjoint operators with non-compact resolvent, in a recent paper [6] Borisov and one of the present authors introduced a new two-dimensional $\mathcal{PT}$-symmetric Hamiltonian with a real continuous spectrum. One of the main questions arising within this model is whether the Hamiltonian possesses point spectrum, too. Using some singular perturbation techniques adopted from the theory of quantum waveguides [13, 5], the question was given both positive and negative answer in [6], depending on the nature of the effective $\mathcal{PT}$-symmetric interaction in a *weakly-coupled* regime. Moreover, in the case when the point spectrum exists, the weakly-coupled eigenvalues emerging from the continuous spectrum were shown to be real. We refer to the next Section 12.2 for a precise statement of the spectral results established in [6].

In the present paper, we further analyse the question of the existence of point spectrum for the Hamiltonian introduced in [6] by *numerical* methods. This enables us to explore quantitative properties of the eigenvalues without the restriction to the weakly-coupled regime. The main emphasis is put on peculiar characteristics of the model which are related to the non-self-adjointness of the underlying Hamiltonian, namely:

1. highly *non-monotone* dependence of the eigenvalues on a coupling parameter; as the parameter increases, the eigenvalues emerge from the continuous spectrum, reach a minimum, sometimes disappear in the continuous spectrum, emerge later on again, *etc*;

2. *broken $\mathcal{PT}$-symmetry*; as the coupling parameter increases, the eigenvalues may emerge from the continuous spectrum as complex-conjugate pairs, collide and become real, move on the real axis, collide again and become complex, *etc.*

This paper is organized as follows. We begin by recalling the Hamiltonian from [6] and summarize the main spectral properties established there. In particular, we point out some questions the study of [6] has left open. In Section 12.3 we describe the numerical methods we use. The numerical data are then presented and discussed in Section 12.4. In the final Section 12.5 we make some conjectures based on the present study.

12.2 The model, known results and open questions

Given a positive number d, we introduce an infinite strip $\Omega := \mathbb{R} \times (0, d)$. We split the variables consistently by writing $x = (x_1, x_2)$ with $x_1 \in \mathbb{R}$ and $x_2 \in (0, d)$. Let $\alpha : \mathbb{R} \to \mathbb{R}$ be a bounded function; occasionally we shall denote by the same symbol the function $x \mapsto \alpha(x_1)$ on Ω. The Hamiltonian H_α we consider in this paper acts simply as the Laplacian in the Hilbert space $L^2(\Omega)$, *i.e.*

$$H_\alpha \Psi := -\Delta\Psi \qquad \text{in} \quad \Omega\,, \tag{12.1}$$

and a non-trivial interaction is introduced by choosing as its domain the set of functions Ψ from $W^{2,2}(\Omega)$ satisfying the following Robin-type boundary conditions:

$$\partial_2\Psi + \mathrm{i}\,\alpha\,\Psi \;=\; 0 \qquad \text{on} \quad \partial\Omega\,. \tag{12.2}$$

Here $W^{2,2}(\Omega)$ denotes the Sobolev space consisting of functions on Ω which, together with all their first and second distributional derivatives, are square integrable. As usual, the action of H_α should be understood in the distributional sense and (12.2) should be understood in the sense of traces [1].

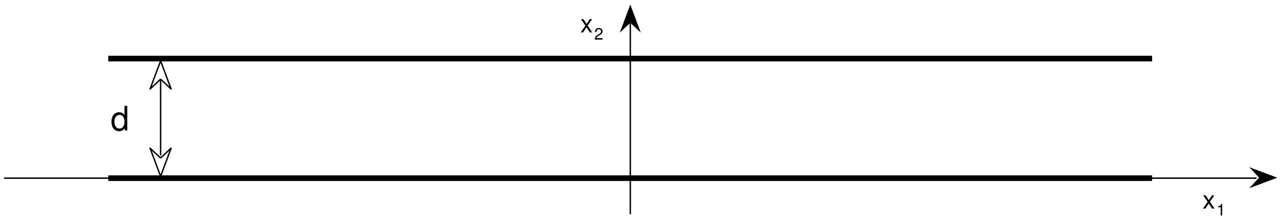

Figure 12.1: A schematic view of an infinite planar waveguide of width d. The Robin conditions (12.2) are imposed at the boundary.

Under the additional hypothesis that α possesses a bounded distributional derivative, *i.e.* $\alpha \in W^{1,\infty}(\mathbb{R})$, it was shown in [6] that H_α is an m-sectorial operator satisfying

$$H_\alpha^* = H_{-\alpha}\,, \tag{12.3}$$

where H_α^* denotes the adjoint of H_α. (If α is merely bounded, it is still possible to give a meaning to H_α by using the quadratic-form approach.) Of course, H_α is not self-adjoint unless α vanishes identically. However, the relation (12.3) reflects the $\mathcal{PT}$-symmetry – or, more generally and more precisely, the $\mathcal{T}$-self-adjointness – of H_α, with $\mathcal{P}$ and $\mathcal{T}$ being defined by $(\mathcal{P}\Psi)(x) := \Psi(d-x)$ and $\mathcal{T}\Psi := \overline{\Psi}$, respectively.

An important property of the operator H_α being m-sectorial is that it is closed. Then, in particular, the spectrum $\sigma(H_\alpha)$ is well defined as the set of complex points z such that $H_\alpha - z$ is not bijective. The point spectrum $\sigma_\mathrm{p}(H_\alpha)$ equals the set of points z such that $H_\alpha - z$ is not injective. The continuous spectrum $\sigma_\mathrm{c}(H_\alpha)$ equals the set of points z such that $H_\alpha - z$ is not surjective but the range of $H_\alpha - z$ is dense in $L^2(\Omega)$. Finally, the residual spectrum $\sigma_\mathrm{r}(H_\alpha)$ equals the set of points z such that $H_\alpha - z$ is injective but the range of $H_\alpha - z$ is not dense in $L^2(\Omega)$.

In the following theorem we collect general results about the spectrum of H_α established in [6]:

Theorem 12.1. *Let $\alpha \in W^{1,\infty}(\mathbb{R})$ and $\alpha_0 \in \mathbb{R}$. Then*

(i) $\sigma(H_\alpha) \subseteq \{z \in \mathbb{C} : |\arg(z)| \leq \theta\}$ *with some* $\theta \in [0, \pi/2)$*;*

(ii) $\sigma_\mathrm{r}(H_\alpha) = \varnothing$*;*

(iii) $\sigma(H_{\alpha_0}) = \sigma_\mathrm{c}(H_{\alpha_0}) = [\mu_0^2, \infty)$ *where* $\mu_0 := \min\{|\alpha_0|, \pi/d\}$*;*

(iv) *if* $\alpha - \alpha_0 \in C_0(\mathbb{R})$*, then* $\sigma_\mathrm{c}(H_\alpha) = [\mu_0^2, \infty)$*;*

(v) *if* $\alpha \in C_0(\mathbb{R})$ *is an odd function, then* $\sigma_\mathrm{p}(H_\alpha) \subset \mathbb{R}$*;*

Here $C_0(\mathbb{R})$ denotes the space of continuous functions on $\mathbb{R}$ with compact support. Note that $\alpha \in C_0(\mathbb{R}) \cap W^{1,\infty}(\mathbb{R})$ implies that α is Lipschitz continuous; conversely, the space of Lipschitz continuous functions on $\mathbb{R}$ is embedded in $W^{1,\infty}(\mathbb{R})$.

The first two properties of Theorem 12.1 are quite general: (i) holds since H_α is sectorial and (ii) is a consequence of the $\mathcal{T}$-self-adjointness (we refer to [6] for more details). Since the spectral problem for the constant case of (iii) can be solved by some sort of "separation of variables" (*cf* [6, Sec. 4]), we shall refer to it as the unperturbed case; it follows from Theorem 12.1 that the corresponding spectrum is purely continuous and positive. As a consequence of (ii), (iv) and (v), we get a result about the reality of the total spectrum in the perturbed case:

Corollary 12.1. *Let $\alpha \in C_0(\mathbb{R}) \cap W^{1,\infty}(\mathbb{R})$ be an odd function. Then*

$$\sigma(H_\alpha) \subset \mathbb{R}\,.$$

The result stated in part (iv) of Theorem 12.1 makes rigorous the heuristic statement that "the continuous spectrum depends on the properties of a Hamiltonian interaction at infinity only". On the other hand, it is well known – and this already for one-dimensional self-adjoint models [17] – that the point spectrum may be highly unstable under a perturbation of an operator with non-compact resolvent. In [6], the point spectrum of H_α was analysed perturbatively in the weakly-coupled regime:

$$\alpha = \alpha_0 + \varepsilon\,\beta\,, \qquad \text{with} \quad \alpha_0 \in \mathbb{R}\,,\ \varepsilon > 0\,,\ \beta \in C_0^2(\mathbb{R})\,, \tag{12.4}$$

where β is assumed to be real-valued and ε plays the role of the small parameter. Here $C_0^2(\mathbb{R})$ denotes the space of functions on $\mathbb{R}$ which, together with all their first and second derivatives, are continuous and have compact support. The main interest was focused on the existence and asymptotic behavior of the eigenvalues emerging from the threshold μ_0^2 of the continuous spectrum due to the perturbation of H_{α_0} by $\varepsilon\beta$.

Before stating the main results of [6] about the weakly-coupled eigenvalues, we need to introduce some notation. Recalling the definition of μ_0 from Theorem 12.1.(iii), we next define

$$\mu_1 := \max\{|\alpha_0|, \pi/d\} \qquad \text{and} \qquad \mu_j := \pi j/d \quad \text{for} \quad j \geq 2\,.$$

To these numbers we associate a family of functions $\{\psi_j\}_{j=0}^\infty$ by

$$\psi_j(x_2) := \cos(\mu_j x_2) - \mathrm{i}\,\frac{\alpha_0}{\mu_j}\,\sin(\mu_j x_2)\,. \tag{12.5}$$

Let $\{v_j\}_{j=0}^\infty$ be a sequence of auxiliary functions given by

$$v_j(x_1) := \begin{cases} -\dfrac{1}{2}\displaystyle\int_{\mathbb{R}} |x_1 - t_1|\beta(t_1)\,dt_1 & \text{if} \quad j = 0\,, \\ \dfrac{1}{2\sqrt{\mu_j^2 - \mu_0^2}}\displaystyle\int_{\mathbb{R}} e^{-\sqrt{\mu_j^2-\mu_0^2}|x_1-t_1|}\beta(t_1)\,dt_1 & \text{if} \quad j \geq 1\,. \end{cases}$$

Finally, denoting $\langle f\rangle = \int_{\mathbb{R}} f(x_1)\,dx_1$ for any $f \in L^1(\mathbb{R})$, we introduce a constant τ, depending on β, d and α_0, by

$$\tau := \begin{cases} 2\alpha_0^2\langle\beta v_0\rangle + \dfrac{2\alpha_0}{d}\displaystyle\sum_{j=1}^\infty \frac{\mu_j^2\langle\beta v_j\rangle}{\mu_j^2 - \mu_0^2}\tan\frac{\alpha_0 d + j\pi}{2} & \text{if} \quad |\alpha_0| < \dfrac{\pi}{d}\,, \\ \dfrac{2\alpha_0\pi^2\cot\frac{\alpha_0 d}{2}}{(\mu_1^2-\mu_0^2)d^3}\langle\beta v_1\rangle + \dfrac{8\pi^2}{(\mu_1^2-\mu_0^2)d^4}\displaystyle\sum_{j=1}^\infty \frac{\mu_{2j}^2\langle\beta v_{2j}\rangle}{\mu_{2j}^2 - \mu_1^2} & \text{if} \quad |\alpha_0| > \dfrac{\pi}{d}\,. \end{cases} \tag{12.6}$$

Now we are in a position to take over from [6]:

Theorem 12.2. *Let α be given by* (12.4)*.*

(A) *If $\alpha_0 = 0$, then H_α has no eigenvalues converging to μ_0^2 as $\varepsilon \to 0$.*

(B) *Let $0 < |\alpha_0| < \pi/d$.*

1. *If $\alpha_0\langle\beta\rangle < 0$, then there exists the unique eigenvalue λ_ε of H_α converging to μ_0^2 as $\varepsilon \to 0$. This eigenvalue is simple and real, and satisfies the asymptotic formula*

$$\lambda_\varepsilon = \mu_0^2 - \varepsilon^2\alpha_0^2\langle\beta\rangle^2 + 2\varepsilon^3\alpha_0\tau\langle\beta\rangle + \mathcal{O}(\varepsilon^4)\,. \tag{12.7}$$

2. *If $\alpha_0\langle\beta\rangle > 0$, then H_α has no eigenvalues converging to μ_0^2 as $\varepsilon \to 0$.*
3. *If $\langle\beta\rangle = 0$ and $\tau > 0$, then there exists the unique eigenvalue λ_ε of H_α converging to μ_0^2 as $\varepsilon \to 0$. This eigenvalue is simple and real, and satisfies the asymptotics*

$$\lambda_\varepsilon = \mu_0^2 - \varepsilon^4\tau^2 + \mathcal{O}(\varepsilon^5)\,. \tag{12.8}$$

4. *If $\langle\beta\rangle = 0$ and $\tau < 0$, then H_α has no eigenvalues converging to μ_0^2 as $\varepsilon \to 0$.*

(C) *Let $|\alpha_0| > \pi/d$ and $\alpha_0 d/\pi \notin \mathbb{Z}$.*

1. *If $\tau > 0$, then there exists the unique eigenvalue λ_ε of H_α converging to μ_0^2 as $\varepsilon \to 0$, it is simple and real, and satisfies the asymptotics* (12.8)*.*
2. *If $\tau < 0$, then H_α has no eigenvalues converging to μ_0^2 as $\varepsilon \to 0$.*

The method of [6] gives also the asymptotic expansion of the eigenfunctions corresponding to the weakly-coupled eigenvalues:

Theorem 12.3. *The eigenfunction Ψ_ε corresponding to any eigenvalue λ_ε from Theorem 12.2 can be chosen so that it satisfies the asymptotics*

$$\Psi_\varepsilon(x) = \psi_0(x_2) + \mathcal{O}(\varepsilon) \tag{12.9}$$

in $W^{2,2}(\Omega \cap \{x : |x_1| < a\})$ for each $a > 0$, and behaves at infinity as

$$\Psi_\varepsilon(x) = \exp^{-\sqrt{\mu_0^2-\lambda_\varepsilon}|x_1|}\,\psi_0(x_2) + \mathcal{O}(\exp^{-\sqrt{\mu_0^2-\lambda_\varepsilon}|x_1|}), \quad x_1 \to +\infty\,. \tag{12.10}$$

Theorems 12.1–12.3 summarizing the spectral analysis performed in [6] leave open the following particular questions:

(Q1) Can the cases (B4) and (C2) of Theorem 12.2 occur? That is, can the constant τ be negative for a certain combination of d, α_0 and β? (Sufficient conditions for the positivity of τ exist [6, Props. 2.1–2.2].)

(Q2) What happens in the case (C) of Theorem 12.2 if the condition $\alpha_0 d/\pi \notin \mathbb{Z}$ is not satisfied? Is it just a technical hypothesis?

(Q3) Is there any point spectrum in the case of Corollary 12.1?

(Q4) What is the dependence of the weakly-coupled eigenvalues of Theorem 12.2 as the parameter ε increases?

(Q5) Do the eigenvalues remain real for large ε?

(Q6) Can one have more eigenvalues? Can they be degenerate? What is the dependence of the number of eigenvalues on ε?

(Q7) Are there any eigenvalues emerging from other thresholds μ_j^2, $j \geq 1$? Can they emerge from other points of the continuous spectrum, different from the thresholds μ_j^2, $j \geq 0$?

The main goal of the present paper is to provide answers to some of these questions by a numerical study of the spectral problem.

12.3 Numerical methods

In order to get the dependence of the bound states on parameters like ε, d, α_0, *etc*, numerically we used two independent methods. When α is a simple step-like function (*e.g.* symmetric or asymmetric square well), we treat the problem by mode matching method. It takes into account the asymptotic behaviour of solution explicitly and can serve thus as a useful check when we apply the other method, *viz.*, the spectral method. This method is more robust and we use it for more general α. We arrived at an excellent agreement in cases when both methods are applicable.

12.3.1 Mode matching method

Let us begin with mode matching. The most general situation we want to describe is shown in Figure 12.2. Fix negative and positive numbers L_- and L_+, respectively. In the asymptotic regions, *i.e.* $x_1 < L_-$ and $L_+ < x_1$, we assume $\alpha(x_1) = \alpha_0$, while in the central parts we have $\alpha(x_1) = \alpha_-$ if $L_- < x_1 < 0$ and $\alpha(x_1) = \alpha_+$ if $0 < x_1 < L_+$.

Let $\{\mu_j^\pm\}_{j=0}^\infty$ denote the sequence of numbers $\{\mu_j\}_{j=0}^\infty$ with α_0 being replaced by $\alpha_\pm$. In the same way we define the sequence of functions $\{\psi_j^\pm\}_{j=0}^\infty$ by replacing α_0 by $\alpha_\pm$ in (12.5). In order to make the notation more consistent, hereafter we write μ_j^0 and ψ_j^0 instead of μ_j and ψ_j, respectively, and introduce a common index $\iota \in \{0, +, -\}$.

In each of the regions where α is constant, the spectral problem $-\Delta\Psi = \lambda\Psi$, with Ψ satisfying the required boundary conditions, can be solved explicitly [6, Sec. 4] by expanding Ψ into the "transverse basis" $\{\psi_j^\iota\}_{j=0}^\infty$,

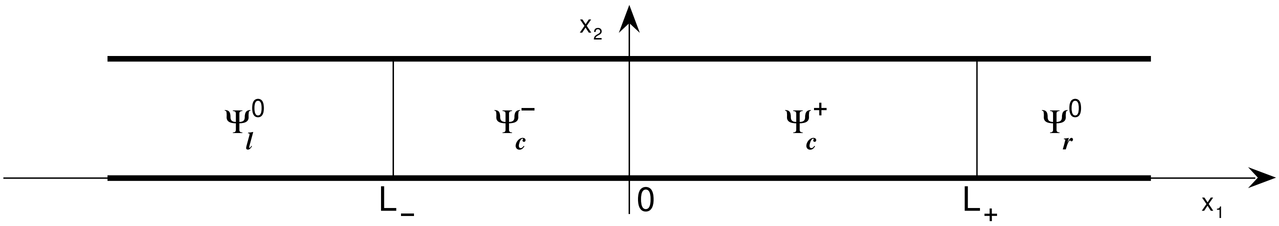

Figure 12.2: The mode matching approach. A particular *Ansatz* (12.11) for an eigenfunction Ψ of H_α corresponding to λ is chosen in each subregion and the smooth matching (12.12) is required at the boundaries separating the subregions.

where ι depends on the region. More specifically, we use the following *Ansatz* for an eigenfunction Ψ of H_α corresponding to λ:

$$\Psi(x) = \begin{cases} \Psi_l^0(x) := \sum_{j=0}^{\infty} d_j \, e^{\sqrt{(\mu_j^0)^2-\lambda}\, x_1}\, \psi_j^0(x_2) & \text{if} \quad x_1 \in (-\infty, L_-)\,, \\ \Psi_c^-(x) := \sum_{j=0}^{\infty} c_j \, \varphi_j^-(x_1)\, \psi_j^-(x_2) & \text{if} \quad x_1 \in (L_-, 0)\,, \\ \Psi_c^+(x) := \sum_{j=0}^{\infty} b_j \, \varphi_j^+(x_1)\, \psi_j^+(x_2) & \text{if} \quad x_1 \in (0, L_+)\,, \\ \Psi_r^0(x) := \sum_{j=0}^{\infty} a_j \, e^{-\sqrt{(\mu_j^0)^2-\lambda}\, x_1}\, \psi_j^0(x_2) & \text{if} \quad x_1 \in (L_+, +\infty)\,, \end{cases} \tag{12.11}$$

where

$$\varphi_j^\pm(x_1) := \cos\left(\sqrt{\lambda - (\mu_j^\pm)^2}\, x_1\right) + B_\pm \sin\left(\sqrt{\lambda - (\mu_j^\pm)^2}\, x_1\right).$$

Standard elliptic regularity theory implies that any weak solution Ψ to $-\Delta\Psi = \lambda\Psi$ is necessarily infinitely smooth in the interior of Ω. In particular, we must match the functions from the *Ansatz* smoothly at $x_1 = L_-, 0, L_+$, *i.e.* we require

$$\begin{aligned} \Psi_l^0(L_-, x_2) &= \Psi_c^-(L_-, x_2)\,, & \partial_1\Psi_l^0(L_-, x_2) &= \partial_1\Psi_c^-(L_-, x_2)\,, \\ \Psi_c^-(0, x_2) &= \Psi_c^+(0, x_2)\,, & \partial_1\Psi_c^-(0, x_2) &= \partial_1\Psi_c^+(0, x_2)\,, \\ \Psi_c^+(L_+, x_2) &= \Psi_r^0(L_+, x_2)\,, & \partial_1\Psi_c^+(L_+, x_2) &= \partial_1\Psi_+^0(L_+, x_2)\,, \end{aligned} \tag{12.12}$$

for every $x_2 \in (0, d)$.

If $\{\psi_j^\iota\}_{j=0}^\infty$ formed an orthonormal family, the next step would consist in employing the orthonormality and reducing (12.12) into a system of algebraic equations for the coefficients a_j, b_j, c_j, d_j. However, since the family $\{\psi_j^\iota\}_{j=0}^\infty$ is actually formed by eigenfunctions of a transverse eigenvalue problem which is not Hermitian (unless $\alpha_\iota = 0$), it is clear that the functions ψ_j^ι are not mutually orthogonal in general. Instead, we use the property that $\{\psi_j^\iota\}_{j=0}^\infty$ and $\{\phi_j^\iota\}_{j=0}^\infty$ form a complete biorthonormal pair [18], where ϕ_j^ι are properly normalized eigenfunctions of the adjoint transverse problem:

$$\phi_j^\iota(x_2) := \overline{A_j^\iota\, \psi_j^\iota(x_2)}\,.$$

The normalization constants can be chosen as follows

$$A_{j_0}^\iota := \frac{2\mathrm{i}\alpha_\iota}{1 - \exp(-2\mathrm{i}\alpha_\iota d)}\,, \quad A_{j_1}^\iota := \frac{2(\mu_1^\iota)^2}{[(\mu_1^\iota)^2 - \alpha_\iota^2]d}\,, \quad A_j^\iota := \frac{2(\mu_j^\iota)^2}{[(\mu_j^\iota)^2 - \alpha_\iota^2]d}\,,$$

where $j \geqslant 2$, $(j_0, j_1) = (0, 1)$ if $|\alpha_\iota| < \pi/d$ and $(j_0, j_1) = (1, 0)$ if $|\alpha_\iota| > \pi/d$ (if $\alpha_\iota = 0$, the fraction in the definition of $A_{j_0}^\iota$ should be understood as the expression obtained after taking the limit $\alpha_\iota \to 0$). Then, in particular, we have

$$\forall i, j \in \mathbb{N}, \quad (\phi_i^\iota, \psi_j^\iota) = \delta_{ij}\,, \tag{12.13}$$

where $(\cdot, \cdot)$ denotes the inner product in $L^2((0, d))$, antilinear in the first factor and linear in the second one.

Now, multiplying (12.12) by $\overline{\phi_i^0}$, integrating over $x_2 \in (0,d)$ and employing (12.13) in the asymptotic regions, we can eliminate the coefficients a_j and d_j by means of the relations

$$\begin{aligned} a_i\, e^{-\sqrt{(\mu_i^0)^2-\lambda}\, L_+} &= \sum_{j=0}^{\infty} b_j\, \varphi_j^+(L_+)\, (\phi_i^0, \psi_j^+)\,, \\ d_i\, e^{\sqrt{(\mu_i^0)^2-\lambda}\, L_-} &= \sum_{j=0}^{\infty} c_j\, \varphi_j^-(L_-)\, (\phi_i^0, \psi_j^-)\,, \end{aligned} \tag{12.14}$$

for every $i \in \mathbb{N}$, and reduce thus the number of conditions to be fulfilled. We finally arrive at an infinite-dimensional homogeneous system

$$\begin{pmatrix} m_{11} & m_{12} & 0 & 0 \\ m_{21} & 0 & m_{23} & 0 \\ 0 & 0 & m_{33} & m_{34} \\ 0 & m_{42} & 0 & m_{44} \end{pmatrix} \begin{pmatrix} b \\ c \\ bB_+ \\ cB_- \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 0 \end{pmatrix}. \tag{12.15}$$

Here b, c denote the infinite vectors formed by b_j, c_j, respectively, and the submatrices $m_{\mu\nu}$ are given by

$$m_{11} := (\phi_i^0, \psi_j^+)\,, \qquad m_{33} := \sqrt{\lambda - (\mu_j^+)^2}\, (\phi_i^0, \psi_j^+)\,,$$

$$m_{12} := -(\phi_i^0, \psi_j^-)\,, \qquad m_{34} := -\sqrt{\lambda - (\mu_j^-)^2}\, (\phi_i^0, \psi_j^-)\,,$$

$$\begin{aligned} m_{21} := \Big(& \sqrt{(\mu_i^0)^2-\lambda}\, \cos\big(L_+\sqrt{\lambda-(\mu_j^+)^2}\big) \\ & - \sqrt{\lambda-(\mu_j^+)^2}\, \sin\big(L_+\sqrt{\lambda-(\mu_j^+)^2}\big)\Big)(\phi_i^0, \psi_j^+)\,, \\ m_{23} := \Big(& \sqrt{(\mu_i^0)^2-\lambda}\, \sin\big(L_+\sqrt{\lambda-(\mu_j^+)^2}\big) \\ & + \sqrt{\lambda-(\mu_j^+)^2}\, \cos\big(L_+\sqrt{\lambda-(\mu_j^+)^2}\big)\Big)(\phi_i^0, \psi_j^+)\,, \\ m_{42} := \Big(& \sqrt{(\mu_i^0)^2-\lambda}\, \cos\big(L_-\sqrt{\lambda-(\mu_j^-)^2}\big) \\ & + \sqrt{\lambda-(\mu_j^-)^2}\, \sin\big(L_-\sqrt{\lambda-(\mu_j^-)^2}\big)\Big)(\phi_i^0, \psi_j^-)\,, \\ m_{44} := \Big(& \sqrt{(\mu_i^0)^2-\lambda}\, \sin\big(L_-\sqrt{\lambda-(\mu_j^-)^2}\big) \\ & - \sqrt{\lambda-(\mu_j^-)^2}\, \cos\big(L_-\sqrt{\lambda-(\mu_j^-)^2}\big)\Big)(\phi_i^0, \psi_j^-)\,, \end{aligned}$$

where the right hand sides should be understood as the infinite matrices formed by the respective coefficients for $i, j \in \mathbb{N}$. Our numerical approximation then consists in approximating the infinite system by using finite submatrices for $i, j \in \{0, \dots, N\}$ with N large enough.

In order to have a nontrivial solution we require

$$\det \begin{pmatrix} m_{11} & m_{12} & 0 & 0 \\ m_{21} & 0 & m_{23} & 0 \\ 0 & 0 & m_{33} & m_{34} \\ 0 & m_{42} & 0 & m_{44} \end{pmatrix} = 0\,, \tag{12.16}$$

which gives an implicit equation for λ as the unknown. Having found λ, we can then calculate the coefficients $a_j, b_j, c_j, d_j, B_{\pm,j}$ from (12.15) and (12.14).

If $\alpha_+ = \alpha_-$ and $L_+ = -L_-$, *i.e.* α is a symmetric square well, then (12.16) can be reduced to

$$\det \begin{pmatrix} m_{21} + m_{42} & 0 \\ 0 & m_{23} - m_{44} \end{pmatrix} = 0\,.$$

The solutions have different symmetry with respect to $x_1 \mapsto -x_1$, the even solutions are formed only of cosines, the odd of sines.

Remark 12.1. In principle, it is possible to extend the present method to an arbitrary piece-wise constant function α, provided that the number of matching interfaces is finite. On the other hand, the more matching conditions the bigger size of the matrix of (12.15) and thus the higher (numerical) price one must pay.

12.3.2 Spectral method

In order to treat the waveguide with a general α in the boundary conditions, we decided to use spectral collocation methods. They provide a reliable and rapidly converging tool easily applicable to our model. A very useful software suite has already been published [26]. It could be adapted to this problem. We approximate the operator by a series of operators defined on a finite domain $[x_1^{min}, x_1^{max}] \times [0, d]$ with Dirichlet boundary conditions on $\{x_1^{min}\} \times [0, d]$ and $\{x_1^{max}\} \times [0, d]$.

First, we can form the differentiation matrices in each variable separately and then combine them to the two-dimensional problem. The infinite domain in x_1-variable suggests that we could approximate it by grid points chosen as the roots of Hermite polynomials and as an interpolant we take Lagrange polynomial. There is an additional parameter (the real line can be mapped to itself by a change of variable $x_1 = b\tilde{x}_1, b > 0$), which can be used to optimize the choice of the grid points together with variation of the number of roots N_1. The roots span the interval $[\xi_1, \xi_{N_1}]$, $-\xi_1 = \xi_{N_1}$, cluster around the origin, and grow as $\xi_{N_1} = \mathcal{O}(\sqrt{N_1})$ for $N_1 \to \infty$.

Another possibility is to use Fourier differencing. We form a uniform grid in $[-x_1^{max}, x_1^{max}]$ and since the solutions decay exponentially, we can theoretically extend it periodically across this interval to the whole $\mathbb{R}$. The interpolant is a trigonometric function.

In both approaches the interpolant is an infinitely differentiable function. Deriving it and taking the derivatives in the grid points we get the differentiation matrices. Imposing the homogeneous Dirichlet boundary conditions consists in deleting the first and the last rows and columns of the differentiation matrices.

The transversal variable is confined to a finite interval $[0, d]$ and it is possible to scale it to $[-1, 1]$. To implement the boundary conditions we prefer to incorporate them into the interpolant. It requires to use Hermite interpolation, which takes into account derivative values in addition to function values. The use of the roots of Chebyshev polynomials $\eta_k = \cos((k-1)\pi/(N_2-1)), k = 1, \ldots, N_2$ as the grid points is common here. For details we refer the reader to [26].

Now, it remains to form differentiation matrices that correspond to partial derivatives entering the Laplacian. Having set up a grid in each direction we combine them into the tensor product grid. Then a closer inspection shows that $\partial_1^2 \to D^{(2)}(x_1) \otimes \mathbf{I}$, where $\mathbf{I}$ is an $N_2 \times N_2$ identity matrix and ∂_2^2 is constructed in a similar way (it is necessary to take into account that the boundary conditions change with x_1).

Applying the spectral discretization we converted the search for eigenvalues of H_α to a matrix eigenvalue problem.

12.4 Discussion of numerical results

Existence of eigenvalues below the threshold of the continuous spectrum and their behaviour for weak perturbations was already proved in [6]. Our calculations confirm it and demonstrate that the spectrum of eigenvalues is considerably richer.

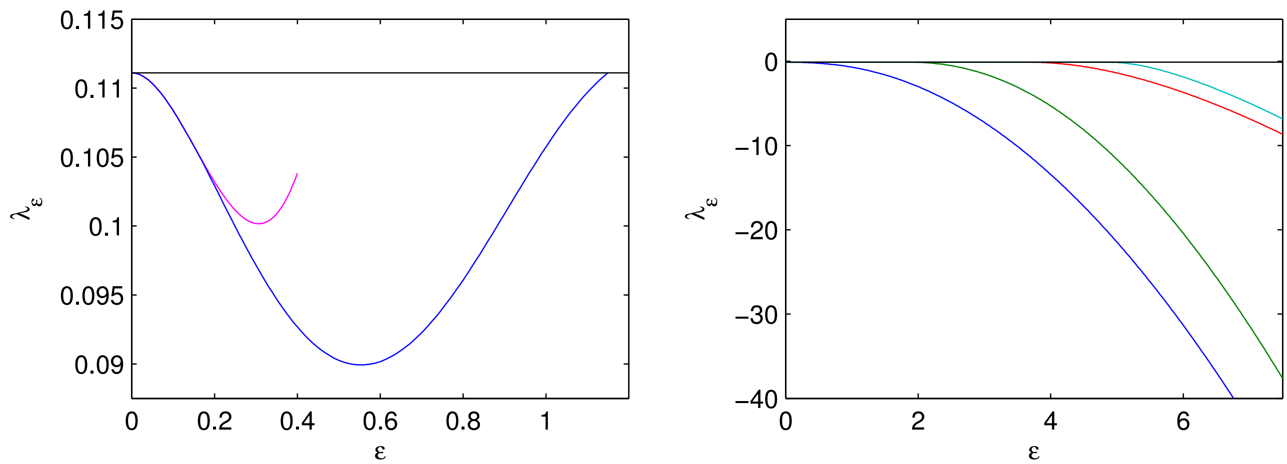

Figure 12.3: Comparison of dependence of eigenvalues on ε for $\mathcal{PT}$-symmetric and self-adjoint waveguides. The left figure shows the $\mathcal{PT}$-symmetric case with $\alpha(x_1) = 1/3 - \varepsilon \exp(-x_1^2)$. Here the blue (respectively magenta) curve represents the eigenvalue (respectively the asymptotic formula (12.7) up to the ε^3-term). The right figure shows the eigencurves in the corresponding self-adjoint situation, obtained by replacing $\mathrm{i}\alpha \mapsto \alpha$ in (12.2). $d = 2$ in both cases.

A typical dependence of an eigenvalue on the perturbation parameter ε is shown in Figure 12.3. Here we perturbed a waveguide of width $d = 2$ and $\alpha_0 = 1/3$ by a Gaussian shape, *i.e.* we took $\beta(x_1) = -\exp(-x_1^2)$

in (12.4). Since $0 < \alpha_0 < \pi/d$ and $\langle\beta\rangle < 0$, we deal with the case (B1) of Theorem 12.2. We observe that the asymptotic expansion (12.7) is fairly good. It is striking, however, that the dependence of the eigenvalue on ε is highly non-monotonic: The eigenvalue appears at some value of ε (in this case it is $\varepsilon = 0$), reaches a minimum, and then returns to the continuous spectrum. We found such a behaviour in all cases we studied, *viz.*, various shapes of symmetric and asymmetric wells, and Gaussians times polynomials. This provides an interesting answer to (Q4) from the end of Section 12.2.

It is worth noting that this behaviour differs from that in the self-adjoint waveguide obtained simply by omitting the imaginary unit in (12.2). As shows the second graph in Figure 12.3, in the self-adjoint case all the energy levels are increasingly more bound when ε increases.

On the other hand, we checked that the eigenvalues are decreasing as functions of $L := \pm L_\pm$ for the symmetric square-well profile $\alpha_+ = \alpha_-$ of Section 12.3.1 in the regime $0 < \alpha_\pm < \alpha_0 < \pi/d$. This is reasonable to expect since as $L \to \infty$ the eigenvalues should approach $(\alpha_\pm)^2$, *i.e.* the threshold of the continuous spectrum of the unperturbed waveguide $H_{\alpha_\pm}$.

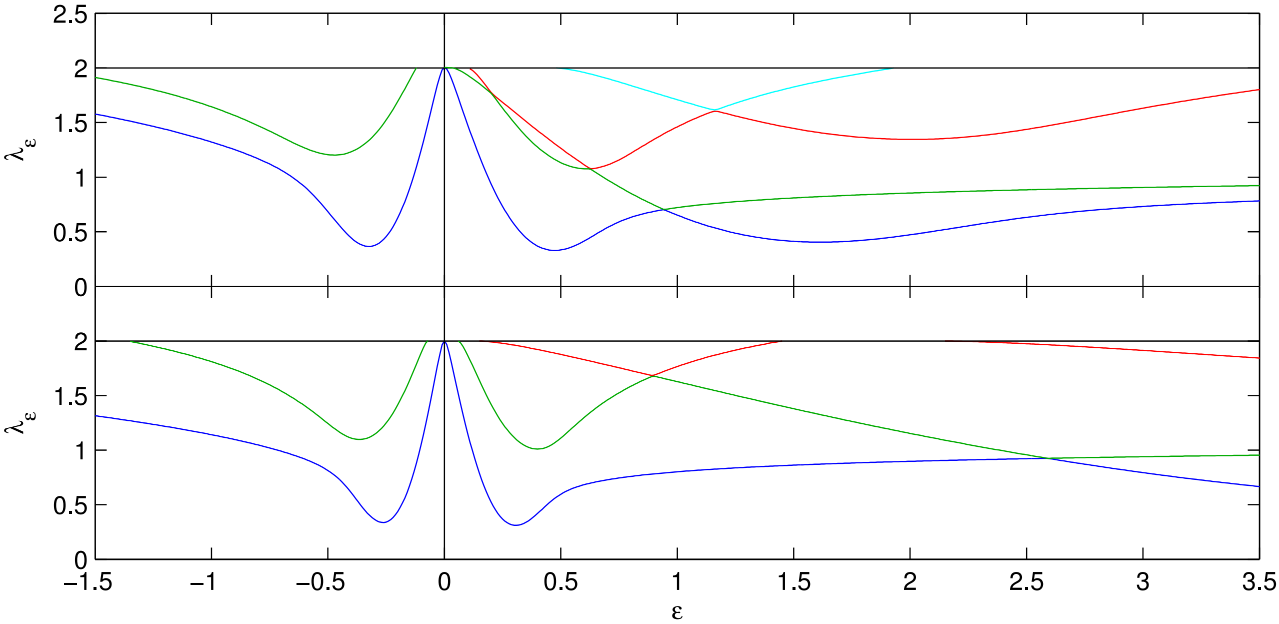

Figure 12.4: Dependence of eigenvalues on ε in the critical case $\langle\beta\rangle = 0$, $\tau > 0$. Here $\alpha(x_1) = \sqrt{2} - \varepsilon(x_1^2 + bx_1 - 5)\exp(-x_1^2/10)$ and $d = 2$. The upper figure corresponds to $b = 1.5$, the lower one to $b = 3.25$. All the crossings are avoided.

An answer to questions from (Q6) is provided by Figure 12.4. It corresponds to the critical case (B3) of Theorem 12.2 with $\beta(x_1) = -(x_1^2 + bx_1 - 5)\exp(-x_1^2/10)$, $\alpha_0 = \sqrt{2}$, and $d = 2$; the parameter b changes the asymmetry of β. In addition to the weakly-coupled eigenvalue of Theorem 12.2, there are also other eigenvalues emerging from the continuous spectrum as ε increases. The lower figure (case $b = 3.25$) shows that there might be eigenvalues existing in disjunct intervals of ε (the red curve). By diminishing α_0 we can achieve the situation when there is only one eigenvalue with a similar behaviour: it emerges from the threshold of continuous spectrum (at $\varepsilon = 0$), reaches a minimum, returns to the continuum, reappears later on, and returns finally to the continuum.

Another typical feature is that the energy levels do not cross. We saw always avoided crossings (at least in the unbroken $\mathcal{PT}$-regime), *i.e.* the order of levels remains unchanged and the non-monotonicity of the excited eigenvalues is preserved.

The spectrum in Figure 12.5 is remarkable from two points of view. First, it corresponds to the case of (Q2) from the end of Section 12.2, since the constant α_0 is chosen so that its square coincides with the threshold of the continuous spectrum, which is $(\pi/2)^2 \approx 2.47$ for $d = 2$. Second, we see that this situation provides a negative answer to (Q5), *i.e.* the $\mathcal{PT}$-symmetry can be broken, and a partial answer to (Q7). Let us comment on the behaviour depicted by the cyan curve. There is a critical value of the parameter ε for which there emerges a pair of complex conjugate eigenvalues from the continuous spectrum (we suspect that they emerge due to a collision of two embedded eigenvalues). As ε increases, the eigenvalues propagate in the complex plane (this is indicated by the curves joining the blue and red dots in the right figure; the dotted curve in the left picture traces the common real parts of the eigencurves) till they collide on the real axis and become real. Then they move on the real axis (as the green dots) in opposite directions till they reach turning points (each of them for

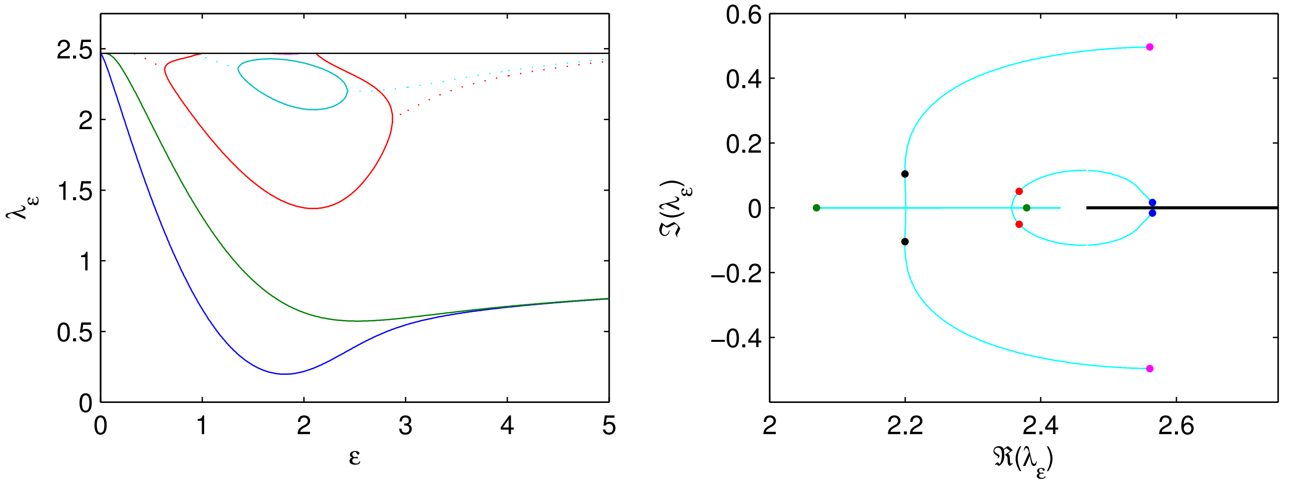

Figure 12.5: Broken $\mathcal{PT}$-symmetry. The left figure shows the dependence of eigenvalues on ε in the case $\alpha(x_1) = \pi/2 - \varepsilon \exp(-x_1^2/10)$ and $d = 2$. Here the dotted line is used to plot the real part of the eigenvalues if they form complex conjugate pairs instead of being real. The right figure shows the trajectory of a pair of (complex) eigenvalues in the complex plane. Here the thick black line marks the continuous spectrum. The pairs of dots show positions of eigenvalues for different values of ε: 0.1 (blue), 1.3 (red), 2.1 (green), 2.5 (black), and 8 (magenta). An animation can be found at the website [19].

different value of ε), starts to approach each other, coalesce again and continue as a pair of complex conjugate eigenvalues (indicated by the black and magenta dots) until they disappear in the continuous spectrum. The behaviour of the eigenvalues depicted by the red curve in the left picture is more difficult in that one of them seems to have the turning point inside the continuous spectrum. Because of the collisions we see that the eigenvalues can actually be degenerate if the $\mathcal{PT}$-symmetry is broken, providing a positive answer to one of the questions from (Q6).

Let us mention that the behaviour of the eigenvalues in the regime of broken $\mathcal{PT}$-symmetry exhibits certain similarities with the over-damped phenomena as regards the spectrum of the infinitesimal generator of the semigroup associated with the damped wave equation [10, 11, 12]. This indicates the unifying framework of Krein spaces behind these two problems [20, 14].

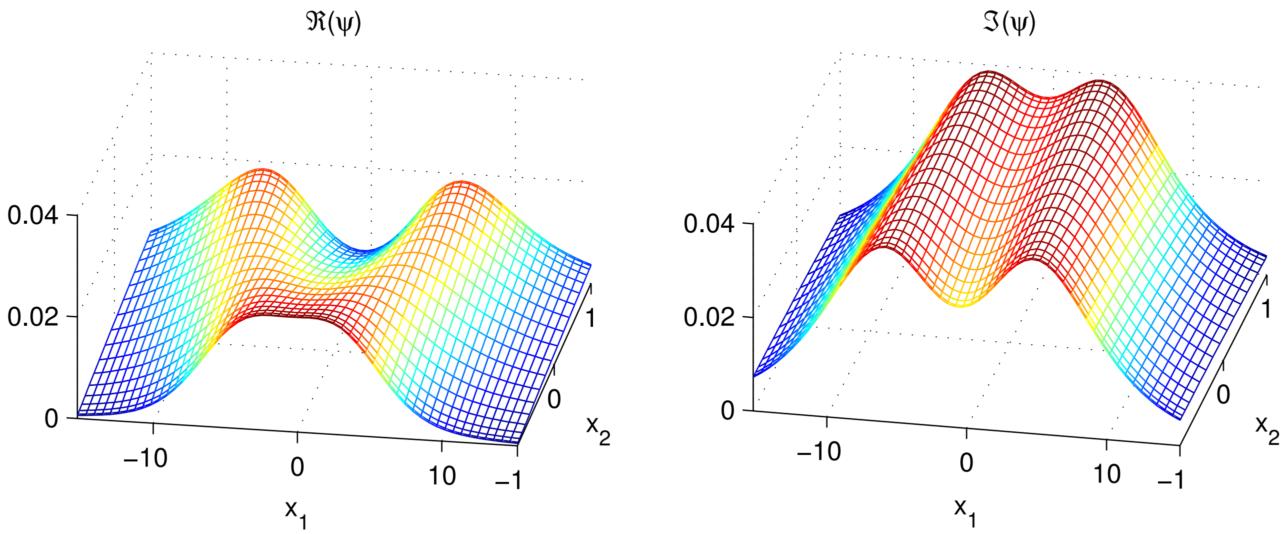

Figure 12.6: Real and imaginary parts of an eigenfunctions corresponding to the smallest (positive) eigenvalue of H_α for $\alpha(x_1) = 1/3 - 0.65 \exp(-0.025 x_1^2)$.

In Figure 12.6, we present an example of eigenfunction corresponding to the case (B1) of Theorem 12.2. We check that the behaviour of the eigenfunction is in perfect agreement with the asymptotic results of Theorem 12.3.

Even if the corresponding eigenenergies are real, the non-Hermiticity prevents from choosing the eigenfunctions real. Since the latter is in particular true for the lowest eigenvalue, it does not make sense to speak about the super- and sub-harmonic properties of the corresponding eigenfunction (which hold in the self-adjoint case). However, although there is no variational characterization of eigenvalues in the present model, numerically we observe that the real and imaginary parts of the eigenfunction corresponding to the lowest eigenvalue are super-harmonic separately in the regime of unbroken $\mathcal{PT}$-symmetry. This follows, of course, from the observations that they do not change sign and that the spectrum is positive.

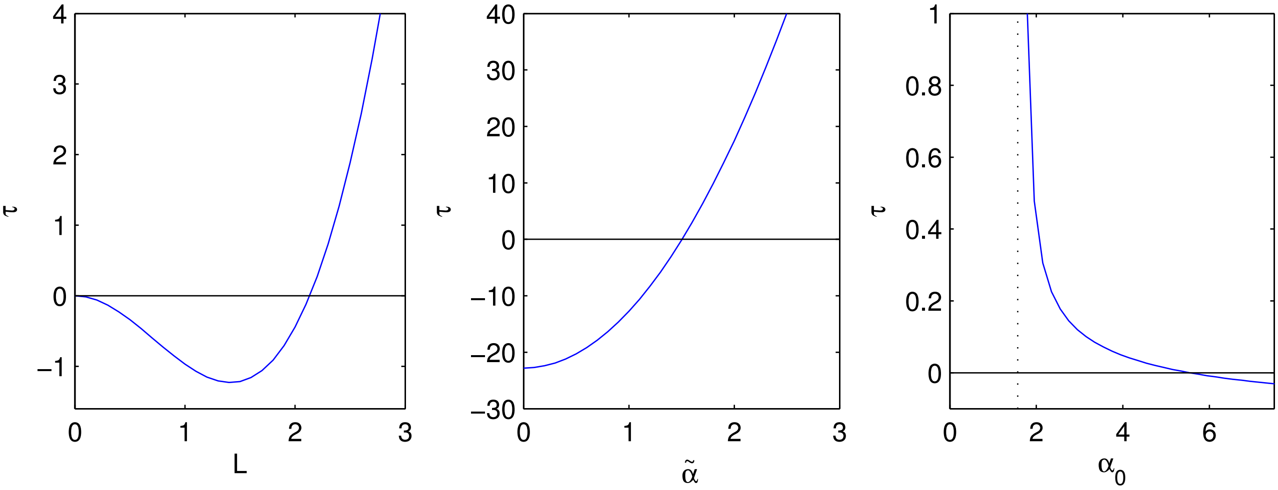

Figure 12.7: Dependence of τ on parameters defining α in the step-like situation of Section 12.3.1, with $d = 2$. The first two figures deal with an antisymmetric square well in the regime $|\alpha_0| < \pi/d$, while the last one deals with a symmetric square well in the regime $\alpha_0 > \pi/d$. The first (respectively second) figure shows the dependence of τ on the width $\pm L_\pm =: L$ (respectively on the coupling $\tilde{\alpha}$) for fixed $\alpha_0 = 1/3$ and $\alpha_\pm = \alpha_0 \mp 1$ (respectively fixed $\alpha_0 = 1$, $\pm L_\pm = 2$ and variable $\alpha_\pm = \alpha_0 \mp \tilde{\alpha}$). In the last figure we show the dependence of τ on α_0 for $L = 10$ and variable $\alpha_\pm = (\alpha_0 - 1)$; here the dotted line corresponds to π/d.

Finally, in Figure 12.7 we visualize the dependence of the complicated quantity τ defined in (12.6) on various parameters. In particular, we see that it changes sign, giving a positive answer to (Q1). Consequently, all the cases of Theorem 12.2 for the critical case $\langle\beta\rangle = 0$ and for the regime $|\alpha_0| > \pi/d$ can be achieved. We also see that the first figure is in qualitative agreement with an analytic result of [6, Prop. 2.1].

12.5 Conclusion

In this paper we tried to enlarge our knowledge of the point spectrum of a non-Hermitian $\mathcal{PT}$-symmetric operator introduced in [6] by analyzing it numerically. We confirmed theoretical results obtained in [6] by perturbation methods, and showed that they actually hold under much milder conditions about α.

Besides this, it turned out that the operator can model a fairly wide range of situations. Indeed, its spectrum is very rich, and certain properties we found are unusual when we compare them with the standard self-adjoint cases. Among them we would like to point out the non-monotonic dependence on the strength of perturbation and the existence of the regime of broken $\mathcal{PT}$-symmetry. We hope that this study will stimulate further theoretical endeavour to extract and prove the salient features.

In particular, based on the present numerical analysis, we conjecture that there will be no other spectrum except for the continuous one if the parameter ε is sufficiently large. At the same time, we were not able to find any discrete eigenvalues in the case of Corollary 12.1, *i.e.* (Q3) from the end of Section 12.2 seems to have a negative answer; the statement (v) of Theorem 12.1 would be trivial, then. Our numerical experiments also indicate that the condition mentioning in (Q2) is indeed just a technical hypothesis in Theorem 12.2.C, in the sense that it does not influence the existence/non-existence of weakly-coupled eigenvalues.

More generally, the existence of eigenvalues in the present model seems to have a nice heuristic explanation. We observe that the discrete spectrum behaves in many respects as that of a one-dimensional Schrödinger operator governed by the first-transverse-eigenvalue potential, *i.e.*, $-\Delta + \min\{\alpha^2, \pi^2/d^2\}$ in $L^2(\mathbb{R})$. Of course, this self-adjoint idealization is just approximative and cannot explain, in particular, the existence of non-real eigenvalues. However, it provides an insight into the non-monotonicity behaviour, the absence of point spectrum for large ε, the positivity of (the real part of) the spectrum, *etc.* It also formally explains the condition from the statement 1 (respectively 2) of Theorem 12.2.B, since this actually implies that the potential is attractive (respectively repulsive).

In this paper we were mainly interested in the eigenvalues emerging from the threshold μ_0^2 of the continuous spectrum. A complete answer to the first question of (Q7) can be provided by a perturbation method similar to that of [6]. However, a more detailed analysis of the continuous spectrum would be still desirable. In particular, Figure 12.4 suggests that there can be embedded eigenvalues for larger values of the coupling parameter.

Finally, let us point out that the question of a direct physical motivation for the Hamiltonian H_α remains open. In this paper we were rather interested in consequences of the non-self-adjointness on spectral properties of this specific model in the context of $\mathcal{PT}$-symmetric quantum mechanics. On the other hand, motivated by problems in semiconductor physics, similar self-adjoint, respectively non-self-adjoint but dissipative, Robin-type boundary conditions has been considered recently in [15], respectively in [16]. In a different context, the present ($\mathcal{PT}$-symmetric) Robin-type boundary conditions imply that we actually deal with the Helmholtz equation in an electromagnetic waveguide with radiation/dissipative boundary conditions.

Acknowledgment

The authors are grateful to Denis Borisov for valuable discussions. The work has been supported by the Czech Academy of Sciences and its Grant Agency within the projects IRP AV0Z10480505 and A100480501, and by the project LC06002 of the Ministry of Education, Youth and Sports of the Czech Republic.

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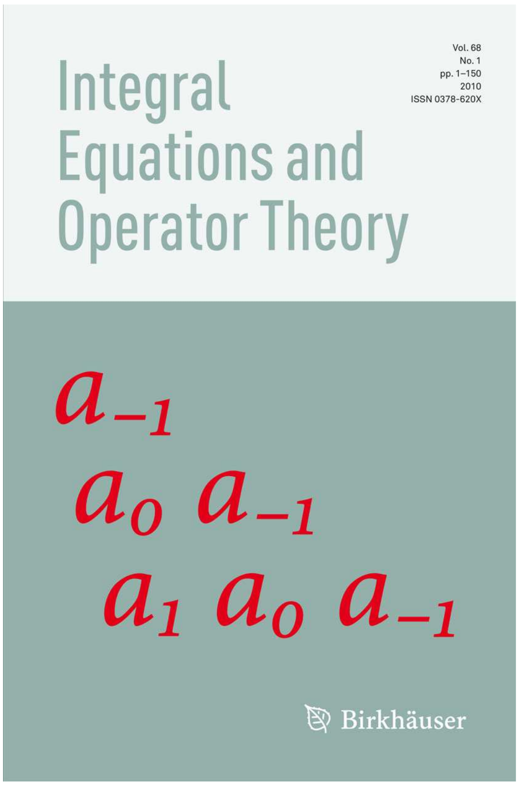
Chapter 13

$\mathcal{PT}$-symmetric waveguides and the lack of variational techniques



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$\mathcal{PT}$-symmetric waveguides and the lack of variational techniques

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Abstract. On a model of waveguide with non-Hermitian Robin-type boundary conditions, we demonstrate the need for a robust method establishing the existence of isolated eigenvalues for non-self-adjoint operators possessing both essential and discrete spectrum.

Mathematics Subject Classification (2010): 35P15, 35J05, 47B44, 81Q12.

Keywords: Robin Laplacian, non-self-adjoint boundary conditions, complex symmetric operator, $\mathcal{PT}$-symmetry, waveguides, discrete and essential spectra.

On the Hilbert space $L^2(\mathbb{R}\times(-1,1))$ let us consider the m-sectorial operator H_α defined as the Laplacian on $H^2(\mathbb{R}\times(-1,1))$, subject to the following complex Robin-type boundary conditions:

$$\frac{\partial\psi}{\partial y} + i\alpha(x)\psi = 0 \qquad \text{for} \qquad (x,y)\in\mathbb{R}\times\{\pm1\}\,,$$

where $\psi \in \mathfrak{D}(H_\alpha)$ and $\alpha : \mathbb{R}\to\mathbb{R}$ is Lipschitz continuous. H_α is not self-adjoint unless $\alpha = 0$, however, it is $\mathcal{T}$-self-adjoint and it commutes with the antilinear product operator $\mathcal{PT}$ where $(\mathcal{P}\psi)(x) := \psi(-x)$ and $(\mathcal{T}\psi)(x) := \overline{\psi(x)}$.

In a joint paper with D. Borisov [1], we performed a detailed spectral analysis of H_α. It was established that the residual spectrum is always empty and that the essential spectrum is real provided that α is a compactly supported perturbation of a constant function α_0:

$$\sigma_{\mathrm{ess}}(H_\alpha) = [\mu_0^2,\infty) \qquad \text{where} \qquad \mu_0 := \min\{|\alpha_0|,\pi/2\}\,.$$

Moreover, assuming that the perturbation $\alpha-\alpha_0$ is small in the supremum norm and using a perturbative method, we derived sufficient conditions for the existence of discrete real weakly-coupled eigenvalues, converging to the threshold μ_0^2 of the essential spectrum when the perturbation vanishes. For instance, one of the sufficient conditions reads

$$|\alpha_0| < \pi/2 \qquad \text{and} \qquad \alpha_0\int_{\mathbb{R}}(\alpha(x)-\alpha_0)\,dx < 0\,,$$

while an opposite sign in the latter inequality ensures that there are no such weakly-coupled eigenvalues.

An open problem is to *show the existence of discrete spectra by some qualitative methods*, regardless of the strength of the perturbation. It is particularly frustrating that the variational techniques powerfully used in self-adjoint waveguides [2] are not available here.

Let us also mention a joint paper with M. Tater [3], where we analysed the spectrum of H_α by numerical methods. It turns out that there might be complex conjugate pairs of discrete eigenvalues if $\alpha-\alpha_0$ is big in the supremum norm [see a related animation (`http://gemma.ujf.cas.cz/~david/KT.html`)]. *Prove this analytically.*

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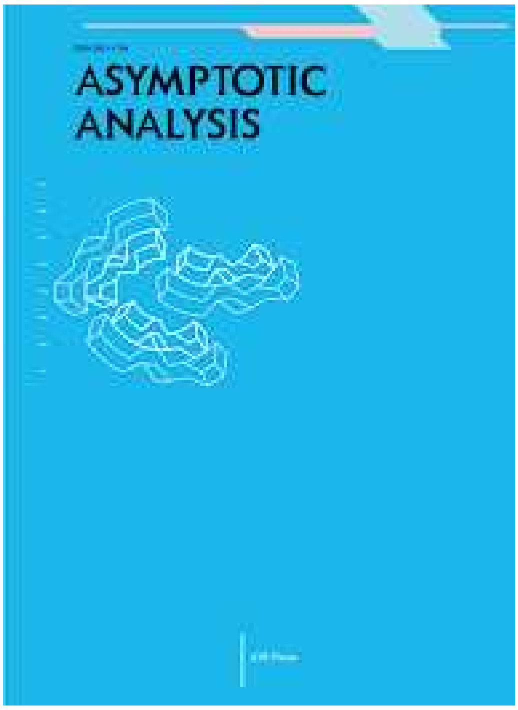
Chapter 14

The effective Hamiltonian for thin layers with non-Hermitian Robin-type boundary conditions



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Joint work with: Denis Borisov

The effective Hamiltonian for thin layers with non-Hermitian Robin-type boundary conditions

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Abstract. The Laplacian in an unbounded tubular neighbourhood of a hyperplane with non-Hermitian complex-symmetric Robin-type boundary conditions is investigated in the limit when the width of the neighbourhood diminishes. We show that the Laplacian converges in a norm resolvent sense to a self-adjoint Schrödinger operator in the hyperplane whose potential is expressed solely in terms of the boundary coupling function. As a consequence, we are able to explain some peculiar spectral properties of the non-Hermitian Laplacian by known results for Schrödinger operators.

14.1 Introduction

There has been a growing interest in spectral properties of differential operators in shrinking tubular neighbourhoods of submanifolds of Riemannian manifolds, subject to various boundary conditions. This is partly motivated by the enormous progress in semiconductor physics, where it is reasonable to try to model a complicated quantum Hamiltonian in a thin nanostructure by an effective operator in a lower dimensional substrate. But the problem is interesting from the purely mathematical point of view as well, because one deals with a singular limit and it is not always obvious how the information about the geometry and boundary conditions are transformed into coefficients of the effective Hamiltonian.

The interest has mainly focused on self-adjoint problems, namely on the Laplacian in the tubular neighbourhoods with uniform boundary conditions of Dirichlet [7, 5, 9, 19] or Neumann [23, 22] or a combination of those [16]. For more references see the review article [12] to which we add the recent works [6, 21] concerned with Robin boundary conditions. The purpose of the present paper is to show that one may obtain an interesting self-adjoint effective operator in the singular limit even if the initial operator is not Hermitian and the geometry is rather trivial.

We consider an operator H_ε which acts as the Laplacian in a d-dimensional layer:

$$H_\varepsilon u = -\Delta u \qquad \text{in} \qquad \Omega_\varepsilon := \mathbb{R}^{d-1} \times (0, \varepsilon)\,, \tag{14.1}$$

where $d \geqslant 2$ and ε is a small positive parameter, subjected to non-Hermitian boundary conditions on $\partial\Omega_\varepsilon$. Instead of considering the general problem, we rather restrict to a special case of separated Robin-type boundary conditions

$$\frac{\partial u}{\partial x_d} + \mathrm{i}\,\alpha(x')\,u = 0 \qquad \text{on} \qquad \partial\Omega_\varepsilon\,, \tag{14.2}$$

where $x = (x_1, \ldots, x_{d-1}, x_d) \equiv (x', x_d)$ denotes a generic point in Ω_ε and α is a real-valued bounded function. More precisely, we consider H_ε as the m-sectorial operator H_ε on $L^2(\Omega_\varepsilon)$ which acts as (14.1) in the distributional sense on the domain consisting of functions u from the Sobolev space $W_2^2(\Omega_\varepsilon)$ satisfying the boundary conditions (14.2). We postpone the formal definition to the following section.

The model H_ε in $d = 2$ was introduced in [4] by the present authors. In that paper, we developed a perturbation theory to study spectral properties of H_ε with ε fixed in the regime when α represents a small and local perturbation of constant α_0 (see below for the discussion of some of the results). Additional spectral properties of H_ε were further studied in [18] by numerical methods. The present paper can be viewed as an addendum by keeping α (and d) arbitrary but sending rather the layer width ε to zero. We believe that the present convergence results provide a valuable insight into the spectral phenomena observed in the two previous papers.

The particular feature of the choice (14.2) is that the boundary conditions are $\mathcal{PT}$-symmetric in the sense that H_ε commutes with the product operator $\mathcal{PT}$. Here $\mathcal{P}$ denotes the parity (space) reversal operator $(\mathcal{P}u)(x) := u(x', \varepsilon - x_d)$ and $\mathcal{T}$ stands for the complex conjugation $(\mathcal{T}u)(x) := \overline{u(x)}$; the latter can be understood as the time reversal operator in the framework of quantum mechanics. The relevance of non-Hermitian $\mathcal{PT}$-symmetric models in physics has been discussed in many papers recently, see the review articles [1, 20]. Non-Hermitian boundary conditions of the type (14.2) were considered in [14] to model open (dissipative) quantum systems.

The role of (14.2) with constant α in the context of perfect-transmission scattering in quantum mechanics is discussed in [13].

Another feature of (14.2) is that the spectrum of H_ε "does not explode" as the layer shrinks, meaning precisely that the resolvent operator $(H_\varepsilon + 1)^{-1}$ admits a non-trivial limit in $L^2(\Omega_\varepsilon)$ as $\varepsilon \to 0$. As a matter of fact, it is the objective of the present paper to show that H_ε converges in a norm resolvent sense to the $(d-1)$-dimensional operator

$$H_0 := -\Delta + \alpha^2 \qquad \text{on} \qquad L^2(\mathbb{R}^{d-1})\,, \tag{14.3}$$

which is a self-adjoint operator on the domain $W_2^2(\mathbb{R}^{d-1})$. Again, we postpone the precise statement of the convergence, which has to take into account that the operators H_ε and H_0 act on different Hilbert spaces, till the following section (*cf* Theorem 14.1). However, let us comment on spectral consequences of the result already now.

First of all, we observe that a significantly non-self-adjoint operator H_ε converges, in the norm resolvent sense, to a self-adjoint Schrödinger operator H_0. The latter contains the information about the non-self-adjoint boundary conditions of the former in a simple potential term. It follows from general facts [15, Sec. IV.3.5] that discrete eigenvalues of H_ε either converge to discrete eigenvalues of H_0 or go to complex infinity or to the essential spectrum of H_0 as $\varepsilon \to \infty$.

In particular, assuming that H_ε and H_0 have the same essential spectrum (independent as a set of ε), the spectrum of H_ε must approach the real axis (or go to complex infinity) in the limit as $\varepsilon \to 0$. Although numerical computations performed in [18] suggest that H_ε might have complex spectra in general, perturbation analysis developed in [4] for the 2-dimensional case shows that both the essential spectrum and weakly coupled eigenvalues are real. The present paper demonstrates that the spectrum is real also as the layer becomes infinitesimally thin, for every $d \geqslant 2$. We would like to stress that the $\mathcal{PT}$-symmetry itself is not sufficient to ensure the reality of the spectrum and that the proof that a non-self-adjoint operator has a real spectrum is a difficult task.

It is also worth noticing that the limiting operator H_0 provides quite precise information about the spectrum of H_ε in the weak coupling regime for $d = 2$ and $|\alpha| < \pi/\varepsilon$ (ε fixed). Indeed, let us consider the following special profile of the boundary function:

$$\alpha_c(x') := \alpha_0 + c\beta(x')\,,$$

where α_0 is a real constant, β is a real-valued function of compact support and c is a real parameter (the regime of weak coupling corresponds to small c). Note that the essential spectrum of both H_ε and H_0 coincides with the interval $[\alpha_0^2, \infty)$, for β is compactly supported (*cf* [4, Thm. 2.2]). It is proved in [4] that if $\alpha_0 \int_{\mathbb{R}} \beta(x')\,dx'$ is negative, then H_ε possesses exactly one discrete real eigenvalue $\mu(c)$ converging to α_0^2 as $c \to 0+$ and the asymptotic expansion

$$\mu(c) = \alpha_0^2 - c^2\,\alpha_0^2 \left(\int_{\mathbb{R}} \beta(x')\,dx' \right)^2 + \mathcal{O}(c^3) \qquad \text{as} \qquad c \to 0+$$

holds true. As a converse result, it is proved in [4] that there is no such a weakly coupled eigenvalue if the quantity $\alpha_0 \int_{\mathbb{R}} \beta(x')\,dx'$ is positive. These weak coupling properties, including the asymptotics above, are well known for the Schrödinger operator H_0 with the potential given by α_c^2, see [10].

At the same time, the form of the potential in H_0 explains some of the peculiar characteristics of H_ε even for large c. As an example, let us recall that a highly non-monotone dependence of the eigenvalues of H_ε on the coupling parameter c was observed in the numerical analysis of [18]. As the parameter increases, a real eigenvalue typically emerges from the essential spectrum, reaches a minimum and then comes back to the essential spectrum again. This behaviour is now easy to understand from the non-linear dependence of the potential α_c^2 on c.

On the other hand, we cannot expect that H_0 represents a good approximation of H_ε for the values of parameters for which H_ε is known to possess complex eigenvalues [18]. It would be then desirable to compute the next to leading term in the asymptotic expansion of H_ε as $\varepsilon \to 0$.

This paper is organized as follows. In Section 14.2 we give a precise definition of the operators H_ε and H_0 and state the norm resolvent convergence of the former to the latter as $\varepsilon \to 0$ (Theorem 14.1). The rest of the paper consists of Section 14.3 in which a proof of the convergence result is given.

14.2 The main result

We start with giving a precise definition of the operators H_ε and H_0.

The limiting operator (14.3) can be immediately introduced as a bounded perturbation of the free Hamiltonian on $L^2(\mathbb{R}^{d-1})$, which is well known to be self-adjoint on the domain $W_2^2(\mathbb{R}^{d-1})$. For later purposes, however, we equivalently understand H_0 as the operator associated on $L^2(\mathbb{R}^{d-1})$ with the quadratic form

$$\begin{aligned} h_0[v] &:= \int_{\mathbb{R}^{d-1}} |\nabla' v(x')|^2 \, dx' + \int_{\mathbb{R}^{d-1}} \alpha(x')^2 \, |v(x')|^2 \, dx', \\ v \in \mathsf{D}(h_0) &:= W_2^1(\mathbb{R}^{d-1}) \, . \end{aligned}$$

Here and in the sequel we denote by ∇' the gradient operator in $\mathbb{R}^{d-1}$, while ∇ stands for the "full" gradient in $\mathbb{R}^d$. Similarly, Δ' denotes the Laplace operator in $\mathbb{R}^{d-1}$.

In the same manner, we introduce H_ε as the m-sectorial operator associated on $L^2(\Omega_\varepsilon)$ with the quadratic form

$$\begin{aligned} h_\varepsilon[u] &:= \int_{\Omega_\varepsilon} |\nabla u(x)|^2 \, dx + \mathrm{i} \int_{\mathbb{R}^{d-1}} \alpha(x') \, |u(x',\varepsilon)|^2 \, dx' - \mathrm{i} \int_{\mathbb{R}^{d-1}} \alpha(x') \, |u(x',0)|^2 \, dx', \\ u \in \mathsf{D}(h_0) &:= W_2^1(\Omega_\varepsilon) \, . \end{aligned}$$

Here the boundary terms are understood in the sense of traces. Note that H_ε is not self-adjoint unless $\alpha = 0$ (in this case H_ε coincides with the Neumann Laplacian in the layer Ω_ε). The adjoint of H_ε is determined by simply changing α to $-\alpha$ (or i to $-$i) in the definition of h_ε. Moreover, H_ε is $\mathcal{T}$-self-adjoint [8, Sec. III.5] (or complex-symmetric [11]), *i.e.* $H_\varepsilon^* = \mathcal{T} H_\varepsilon \mathcal{T}$.

The form h_ε is well defined under the mere condition that α is bounded. However, if we strengthen the regularity to $\alpha \in W_\infty^1(\mathbb{R}^{d-1})$, it can be shown by standard procedures (*cf* [4, Sec. 3]) that H_ε coincides with the operator described in the introduction, *i.e.*, it acts as the (distributional) Laplacian (14.1) on the domain formed by the functions u from $W_2^2(\Omega_\varepsilon)$ satisfying the boundary conditions (14.2) in the sense of traces.

The operator H_0 is clearly non-negative. An analogous property for H_ε is contained in the following result

$$\sigma(H_\varepsilon) \subset \Big\{ z \in \mathbb{C} \ \Big| \ \operatorname{Re} z \geqslant 0, \, |\operatorname{Im} z| \leqslant 2 \, \|\alpha\|_\infty \sqrt{\operatorname{Re} z} \Big\} \, . \tag{14.4}$$

Here and in the sequel we denote by $\|\cdot\|_\infty$ the supremum norm. (14.4) can be proved exactly in the same way as in [4, Lem. 3.1] for $d = 2$ by estimating the numerical range of H_ε. In particular, the open left half-plane of $\mathbb{C}$ belongs to the resolvent set of both H_ε and H_0.

Another general spectral property of H_ε, common with H_0, is that its residual spectrum is empty. This is a consequence of the $\mathcal{T}$-self-adjointness property of H_ε as pointed out in [4, Corol. 2.1].

Since H_ε and H_0 act on different Hilbert spaces, we need to explain how the convergence of the corresponding resolvent operators is understood. We are inspired by [9]. We decompose our Hilbert space into an orthogonal sum

$$L^2(\Omega_\varepsilon) = \mathfrak{H}_\varepsilon \oplus \mathfrak{H}_\varepsilon^\perp \, , \tag{14.5}$$

where the subspace $\mathfrak{H}_\varepsilon$ consists of functions from $L^2(\Omega_\varepsilon)$ of the form $x \mapsto \psi(x')$, *i.e.* independent of the "transverse" variable x_d. The corresponding projection is given by

$$(P_\varepsilon u)(x) := \frac{1}{\varepsilon} \int_0^\varepsilon u(x) \, \mathrm{d}x_d \tag{14.6}$$

and it can be viewed as a projection onto a constant function in the transverse variable. We also write $P_\varepsilon^\perp := I - P_\varepsilon$. Since the functions from $\mathfrak{H}_\varepsilon$ depend on the "longitudinal" variables x' only, $\mathfrak{H}_\varepsilon$ can be naturally identified with $L^2(\mathbb{R}^{d-1})$. More precisely, the identity mapping $u \mapsto u$ represents the isometric isomorphism between $\mathfrak{H}_\varepsilon$ and $L^2(\mathbb{R}^{d-1})$. Hence, with an abuse of notations, we may identify any operator on $L^2(\mathbb{R}^{d-1})$ as the operator acting on the subspace $\mathfrak{H}_\varepsilon \subset L^2(\Omega_\varepsilon)$, and vice versa.

The norm and the inner product in $L^2(\Omega_\varepsilon)$ will be denoted by $\|\cdot\|_\varepsilon$ and $(\cdot,\cdot)_\varepsilon$, respectively. We keep the same notation $\|\cdot\|_\varepsilon$ for the operator norm on $L^2(\Omega_\varepsilon)$. The norm and the inner product in $L^2(\mathbb{R}^{d-1})$ will be denoted by $\|\cdot\|$ and $(\cdot,\cdot)$, respectively, *i.e.* without the subscript ε. All the inner products are assumed to be linear in the first component. Finally, we denote the norm in $W_2^1(\Omega_\varepsilon)$ by $\|\cdot\|_{\varepsilon,1}$ and we keep the same notation for the norm of bounded operators from $L_2(\Omega_\varepsilon)$ to $W_2^1(\Omega_\varepsilon)$.

Now we are in a position to formulate the main result of this paper.

Theorem 14.1. *Assume $\alpha \in W_\infty^1(\mathbb{R}^{d-1})$. Then the inequalities*

$$\big\|(H_\varepsilon + 1)^{-1} - (H_0 + 1)^{-1} P_\varepsilon\big\|_\varepsilon \leqslant C \, \varepsilon, \tag{14.7}$$

$$\big\|(H_\varepsilon + 1)^{-1} - (1 + Q)(H_0 + 1)^{-1} P_\varepsilon\big\|_{\varepsilon,1} \leqslant C(\varepsilon) \, \varepsilon \tag{14.8}$$

hold true, where $Q(x) := -\mathrm{i}\,\alpha(x')\,x_d$ *and*

$$C := \sqrt{\frac{1}{\pi^2} + \frac{(\|\nabla'\alpha\|_\infty + 2\|\alpha\|_\infty)^2}{3}}\,,$$

$$C(\varepsilon) := \sqrt{\frac{1}{\pi^2} + \left(\frac{\|\nabla'\alpha\|_\infty + \|\alpha\|_\infty}{\sqrt{3}} + C_1(\varepsilon)\right)^2}\,,$$

$$C_1(\varepsilon) := \sqrt{\left(\frac{\varepsilon\|\alpha\|_\infty^2}{2\sqrt{5}}\right)^2 + \left(\frac{\varepsilon\|\alpha\|_\infty^2}{2\sqrt{5}} + \frac{\|\alpha\|_\infty\sqrt{\|\alpha\|_\infty^2 + \|\nabla'\alpha\|_\infty^2\,\varepsilon^2}}{\sqrt{3}}\right)^2}\,.$$

Let us discuss the result of this theorem. It says that the operator H_ε converges to H_0 in the norm resolvent sense. Note that, contrary to what happens for instance in the case of uniform Dirichlet boundary conditions, here we can choose the spectral parameter fixed (*e.g.* $-1 \in \rho(H_\varepsilon) \cap \rho(H_0)$ as in the theorem) and still get a non-trivial result.

If we treat the convergence of the resolvents in the topology of bounded operators in $L_2(\Omega_\varepsilon)$, the estimate (14.7) says that the rate of the convergence is of order $\mathcal{O}(\varepsilon)$. At the same time, if we consider the convergence as for the operators acting from $L_2(\Omega_\varepsilon)$ into $W_2^1(\Omega_\varepsilon)$, to keep the same rate of the convergence, one has to use the function Q. This functions is to be understood as a corrector needed to have the convergence in a stronger norm. Such situation is well-known and it often happens for singularly perturbed problems, especially in the homogenization theory, see, *e.g.*, [3, 2, 24].

Remark 14.1. For twice differentiable α, the unitary transform on $L^2(\Omega_\varepsilon)$ generated by the multiplication operator $x \mapsto e^{\mathrm{i}\alpha(x')x_d}$ enables one to transfer the boundary conditions (14.2) into coefficients of the operator unitarily equivalent to the Robin Laplacian (*cf* [17, Sec. 6.1]). More specifically, the unitarily equivalent operator acts as a Schrödinger-type operator with complex coefficients

$$-\Delta - 2i\begin{pmatrix} x_d\nabla'\alpha \\ \alpha \end{pmatrix}\cdot\nabla + x_d^2|\nabla'\alpha|^2 - ix_d\,\Delta'\alpha + \alpha^2 \tag{14.9}$$

and satisfies the usual Neumann boundary conditions on $L^2(\Omega_\varepsilon)$. This idea has been employed previously in [4, Sec. 6] to study the discrete spectrum of H_ε. Here we do not follow this approach in order to avoid imposing additional regularity assumptions about α. However, (14.9) is instructive in order to guess the form of the limiting operator (14.3). Indeed, projecting (14.9) onto the constant transverse mode and sending ε to zero (recall $x_d \in (0,\varepsilon)$), (14.9) formally converges to (14.3).

Remark 14.2. Theorem 14.1 is formulated in terms of ε-dependent norms. It is also possible to reformulate the main result in fixed norms, if one employs the unitary transformation $u(x) \mapsto \varepsilon^{-1/2}\,u(x', \varepsilon^{-1}x_d) =: v(x', x_d)$. Under such transformation, the domain Ω_ε rescales to Ω_1 and the operator H_ε is unitarily equivalent to

$$\widetilde{H}_\varepsilon := -\Delta' - \varepsilon^{-2}\,\partial_d^2 \qquad \text{on} \qquad L^2(\Omega_1)\,,$$

subject to the boundary conditions $\partial_d v + \varepsilon\,\mathrm{i}\,\alpha(x')\,v = 0$. The estimate (14.7) casts into the equivalent form

$$\big\|(\widetilde{H}_\varepsilon + 1)^{-1} - (H_0 + 1)^{-1}P_1\big\|_1 \leqslant C\,\varepsilon\,,$$

while the next one becomes more complicated and this is why we do not give it here.

14.3 Proof of Theorem 14.1

Throughout this section we assume $\alpha \in W_\infty^1(\mathbb{R}^{d-1})$. With an abuse of notation, we denote by the same symbol α both the function on $\mathbb{R}^{d-1}$ and its natural extension $x \mapsto \alpha(x')$ to $\mathbb{R}^d$.

We start with two auxiliary lemmata. The first tells us that the subspace $\mathfrak{H}_\varepsilon^\perp$ is negligible for H_ε in the limit as $\varepsilon \to 0$.

Lemma 14.1. *For any* $f \in L^2(\Omega_\varepsilon)$*, we have*

$$\big\|(H_\varepsilon + 1)^{-1}P_\varepsilon^\perp f\big\|_{\varepsilon,1} \leqslant \frac{\varepsilon}{\pi}\,\|P_\varepsilon^\perp f\|_\varepsilon\,. \tag{14.10}$$

Proof. For any fixed $f \in L^2(\Omega_\varepsilon)$, let us set $u := (H_\varepsilon + 1)^{-1}P_\varepsilon^\perp f \in \mathsf{D}(H_\varepsilon) \subset W_2^1(\Omega_\varepsilon)$. In other words, u satisfies the resolvent equation

$$\forall v \in W_2^1(\Omega_\varepsilon)\,, \qquad h_\varepsilon(u,v) + (u,v)_\varepsilon = (P_\varepsilon^\perp f, v)_\varepsilon\,,$$

where $h_\varepsilon(\cdot,\cdot)$ denotes the sesquilinear form associated with the quadratic form $h_\varepsilon[\cdot]$. Choosing u for the test function v and taking the real part of the obtained identity, we get

$$\|u\|_{\varepsilon,1}^2 = \operatorname{Re}\left(P_\varepsilon^\perp f, u\right)_\varepsilon = \operatorname{Re}\left(P_\varepsilon^\perp f, P_\varepsilon^\perp u\right)_\varepsilon \leqslant \|P_\varepsilon^\perp f\|_\varepsilon \|P_\varepsilon^\perp u\|_\varepsilon . \tag{14.11}$$

Employing the decomposition $u = P_\varepsilon u + P_\varepsilon^\perp u$, the left hand side of (14.11) can be estimated as follows

$$\|u\|_{\varepsilon,1}^2 \geqslant \|\nabla u\|_\varepsilon^2 \geqslant \|\partial_d u\|_\varepsilon^2 = \|\partial_d P_\varepsilon^\perp u\|_\varepsilon^2 \geqslant (\pi/\varepsilon)^2 \|P_\varepsilon^\perp u\|_\varepsilon^2 . \tag{14.12}$$

Here the last inequality follows from the variational characterization of the second eigenvalue of the Neumann Laplacian on $L^2((0,\varepsilon))$ and Fubini's theorem. Combining (14.12) with (14.11), we obtain

$$\|P_\varepsilon^\perp u\|_\varepsilon \leqslant (\varepsilon/\pi)^2 \|P_\varepsilon^\perp f\|_\varepsilon .$$

Finally, applying the obtained inequality to the right hand side of (14.11), we conclude with

$$\|u\|_{\varepsilon,1}^2 \leqslant (\varepsilon/\pi)^2 \|P_\varepsilon^\perp f\|_\varepsilon^2 .$$

This is equivalent to the estimate (14.10). □

In the second lemma we collect some elementary estimates we shall need later on.

Lemma 14.2. *We have*

$$|\mathrm{e}^{-\mathrm{i}\alpha x_d} - 1| \leqslant \|\alpha\|_\infty x_d , \tag{14.13}$$

$$|\mathrm{e}^{-\mathrm{i}\alpha x_d} - 1 + \mathrm{i}\alpha x_d| \leqslant \frac{1}{2} \|\alpha\|_\infty^2 x_d^2 , \tag{14.14}$$

$$|\nabla(\mathrm{e}^{-\mathrm{i}\alpha x_d} - 1 + \mathrm{i}\alpha x_d)| \leqslant \|\alpha\|_\infty x_d \sqrt{\|\alpha\|_\infty^2 + \|\nabla'\alpha\|_\infty^2 x_d^2} . \tag{14.15}$$

Proof. The estimates (14.13) and (14.14) are elementary and we leave the proofs to the reader. The last estimate (14.15) follows from (14.13) and the identity

$$\nabla(\mathrm{e}^{-\mathrm{i}\alpha x_d} - 1 + \mathrm{i}\alpha x_d) = \mathrm{i}(1 - \mathrm{e}^{-\mathrm{i}\alpha x_d}) \begin{pmatrix} x_d \nabla'\alpha \\ \alpha \end{pmatrix}$$

taken into account. □

We continue with the proof of Theorem 14.1. Let $f \in L^2(\Omega_\varepsilon)$. Accordingly to (14.5), f admits the decomposition $f = P_\varepsilon f + P_\varepsilon^\perp f$ and we have

$$\|f\|_\varepsilon^2 = \|P_\varepsilon f\|_\varepsilon^2 + \|P_\varepsilon^\perp f\|_\varepsilon^2 = \varepsilon \|P_\varepsilon f\|^2 + \|P_\varepsilon^\perp f\|_\varepsilon^2 . \tag{14.16}$$

We define $u := (H_\varepsilon + 1)^{-1} f$ and make the decomposition

$$u = u_0 + u_1 \qquad \text{with} \qquad u_0 := (H_\varepsilon + 1)^{-1} P_\varepsilon f , \quad u_1 := (H_\varepsilon + 1)^{-1} P_\varepsilon^\perp f . \tag{14.17}$$

In view of Lemma 14.1, u_1 is negligible in the limit as $\varepsilon \to 0$,

$$\|u_1\|_{\varepsilon,1} \leqslant \frac{\varepsilon}{\pi} \|P_\varepsilon^\perp f\|_\varepsilon . \tag{14.18}$$

It remains to study the dependence of u_0 on ε. We construct u_0 as follows

$$u_0(x) = \mathrm{e}^{-\mathrm{i}\alpha(x')x_d} w_0(x') + w_1(x) , \qquad \text{where} \qquad w_0 := (H_0 + 1)^{-1} P_\varepsilon f \tag{14.19}$$

and w_1 is a function defined by this decomposition.

First, we establish a rather elementary bound for w_0.

Lemma 14.3. *We have*

$$\|w_0\|_{\varepsilon,1} \leqslant \|P_\varepsilon f\|_\varepsilon .$$

Proof. By definition, w_0 satisfies the resolvent equation

$$\forall v \in W_2^1(\mathbb{R}^{d-1}), \qquad h_0(w_0, v) + (w_0, v) = (P_\varepsilon f, v), \tag{14.20}$$

where $h_0(\cdot,\cdot)$ denotes the sesquilinear form associated with the quadratic form $h_0[\cdot]$. Choosing w_0 for the test function v, we get

$$\|\nabla' w_0\|^2 + \|\alpha w_0\|^2 + \|w_0\|^2 = (P_\varepsilon f, w_0) \leqslant \|P_\varepsilon f\| \|w_0\|. \tag{14.21}$$

In particular,

$$\|w_0\| \leqslant \|P_\varepsilon f\|.$$

Using this estimate in the right hand side of (14.21), we get

$$\|\nabla' w_0\|^2 + \|w_0\|^2 \leqslant \|P_\varepsilon f\|^2.$$

Reintegrating this inequality over $(0, \varepsilon)$, we conclude with the desired bound in Ω_ε. □

It is more difficult to get a bound for w_1.

Lemma 14.4. *We have*

$$\|w_1\|_{\varepsilon,1} \leqslant C_0\, \varepsilon\, \|P_\varepsilon f\|_\varepsilon \qquad \text{with} \qquad C_0 := \frac{\|\nabla' \alpha\|_\infty + \|\alpha\|_\infty}{\sqrt{3}}.$$

Proof. By definition, u_0 satisfies the resolvent equation

$$\forall v \in W_2^1(\Omega_\varepsilon), \qquad h_\varepsilon(u_0, v) + (u_0, v)_\varepsilon = (P_\varepsilon f, v)_\varepsilon.$$

Choosing w_1 for the test function v and using the decomposition (14.19), we get

$$h_\varepsilon[w_1] + \|w_1\|_\varepsilon^2 = (P_\varepsilon f, w_1)_\varepsilon - h_\varepsilon(u_0 - w_1, w_1) - (u_0 - w_1, w_1)_\varepsilon =: F_\varepsilon. \tag{14.22}$$

It is straightforward to check that

$$\begin{aligned} h_\varepsilon(u_0 - w_1, w_1) &= \big(\nabla w_0, \nabla e^{\mathrm{i}\alpha x_d} w_1\big)_\varepsilon + \big(\alpha^2 w_0, e^{\mathrm{i}\alpha x_d} w_1\big)_\varepsilon - F'_\varepsilon \\ &= -\big(w_0, e^{\mathrm{i}\alpha x_d} w_1\big)_\varepsilon + \big(P_\varepsilon f, e^{\mathrm{i}\alpha x_d} w_1\big)_\varepsilon - F'_\varepsilon \end{aligned}$$

with

$$F'_\varepsilon := \mathrm{i}\big(x_d\, w_0\, \nabla' \alpha, \mathrm{e}^{\mathrm{i}\alpha x_d} \nabla' w_1\big)_\varepsilon - \mathrm{i}\big(\nabla' w_0, x_d\, e^{\mathrm{i}\alpha x_d} w_1\, \nabla' \alpha\big)_\varepsilon.$$

Here the first equality follows by algebraic manipulations using an integration by parts, while the second is a consequence of (14.20), with $x' \mapsto e^{\mathrm{i}\alpha(x')x_d} w_1(x', x_d)$ being the test function, and Fubini's theorem. At the same time, $(u_0 - w_1, w_1)_\varepsilon = (w_0, e^{\mathrm{i}\alpha x_d} w_1)_\varepsilon$. Hence,

$$F_\varepsilon = F'_\varepsilon + \big(P_\varepsilon f, w_1 - e^{\mathrm{i}\alpha x_d} w_1\big)_\varepsilon.$$

We proceed with estimating F_ε:

$$\begin{aligned} |F_\varepsilon| &\leqslant \frac{\varepsilon^{3/2}}{\sqrt{3}} \Big(\|\nabla' \alpha\|_\infty \|w_0\| \|\nabla' w_1\|_\varepsilon + \|\nabla' \alpha\|_\infty \|\nabla' w_0\| \|w_1\|_\varepsilon + \|\alpha\|_\infty \|P_\varepsilon f\| \|w_1\|_\varepsilon \Big) \\ &\leqslant \frac{\varepsilon^{3/2}}{\sqrt{3}} \Big(\|\nabla' \alpha\|_\infty \sqrt{\|w_0\|^2 + \|\nabla' w_0\|^2} \sqrt{\|\nabla' w_1\|_\varepsilon^2 + \|w_1\|_\varepsilon^2} + \|\alpha\|_\infty \|P_\varepsilon f\| \|w_1\|_\varepsilon \Big) \\ &\leqslant \frac{\varepsilon}{\sqrt{3}} \Big(\|\nabla' \alpha\|_\infty \|w_0\|_{\varepsilon,1} + \|\alpha\|_\infty \|P_\varepsilon f\|_\varepsilon \Big) \|w_1\|_{\varepsilon,1}. \end{aligned}$$

Here the first inequality follows by the Schwarz inequality, an explicit value of the integral of x_d^2 and obvious bounds such as (14.13).

Finally, taking the real part of (14.22) and using the above estimate of $|F_\varepsilon|$, we get

$$\|w_1\|_{\varepsilon,1} \leqslant \frac{\varepsilon}{\sqrt{3}} \Big(\|\nabla' \alpha\|_\infty \|w_0\|_{\varepsilon,1} + \|\alpha\|_\infty \|P_\varepsilon f\|_\varepsilon \Big).$$

The desired bound then follows by estimating $\|w_0\|_{\varepsilon,1}$ by means of Lemma 14.3. □

Now we are in a position to conclude the proof of Theorem 14.1 by simply comparing u with w_0. As for the convergence in the topology of $L^2(\Omega_\varepsilon)$, we write

$$\begin{aligned}\|u-w_0\|_\varepsilon &= \|u_1+w_1+(\mathrm{e}^{-\mathrm{i}\alpha x_d}-1)w_0\|_\varepsilon \\ &\leqslant \|u_1\|_\varepsilon+\|w_1\|_\varepsilon+\|(\mathrm{e}^{-\mathrm{i}\alpha x_d}-1)w_0\|_\varepsilon .\end{aligned}$$

Here the last term can be estimated using Lemma 14.2 as follows

$$\|(\mathrm{e}^{-\mathrm{i}\alpha x_d}-1)w_0\|_\varepsilon \leqslant \frac{\varepsilon^{3/2}}{\sqrt{3}}\,\|\alpha\|_\infty\|w_0\| = \frac{\varepsilon}{\sqrt{3}}\,\|\alpha\|_\infty\|w_0\|_\varepsilon .$$

Hence, using (14.18), Lemma 14.4 and Lemma 14.3, we get the bound

$$\begin{aligned}\|u-w_0\|_\varepsilon &\leqslant \|u_1\|_{\varepsilon,1}+\|w_1\|_{\varepsilon,1}+\frac{\varepsilon}{\sqrt{3}}\,\|\alpha\|_\infty\|w_0\|_\varepsilon \\ &\leqslant \varepsilon\left(\frac{1}{\pi}\,\|P_\varepsilon^\perp f\|_\varepsilon+\frac{1}{\sqrt{3}}\big(\|\nabla'\alpha\|_\infty+2\,\|\alpha\|_\infty\big)\,\|P_\varepsilon f\|_\varepsilon\right) \\ &\leqslant C\,\varepsilon\,\|f\|_\varepsilon\end{aligned}$$

Here the last estimate follows by the Schwarz inequality recalling (14.16) and holds with the constant C as defined in Theorem 14.1. This proves (14.7).

As for the bound (14.8), we have

$$\begin{aligned}\|u-(1+Q)w_0\|_{\varepsilon,1} &= \|u_1+w_1+(\mathrm{e}^{-\mathrm{i}\alpha x_d}-1+\mathrm{i}\alpha x_d)w_0\|_{\varepsilon,1} \\ &\leqslant \|u_1\|_{\varepsilon,1}+\|w_1\|_{\varepsilon,1}+\|(\mathrm{e}^{-\mathrm{i}\alpha x_d}-1+\mathrm{i}\alpha x_d)w_0\|_{\varepsilon,1} .\end{aligned}$$

Here the last term can be estimated using Lemma 14.2 as follows. Employing the individual estimates

$$\begin{aligned}\|(\mathrm{e}^{-\mathrm{i}\alpha x_d}-1+\mathrm{i}\alpha x_d)w_0\|_\varepsilon &\leqslant \frac{\varepsilon^{5/2}}{2\sqrt{5}}\,\|\alpha\|_\infty^2\|w_0\| = \frac{\varepsilon^2}{2\sqrt{5}}\,\|\alpha\|_\infty^2\|w_0\|_\varepsilon , \\ \|(\mathrm{e}^{-\mathrm{i}\alpha x_d}-1+\mathrm{i}\alpha x_d)\nabla w_0\|_\varepsilon &\leqslant \frac{\varepsilon^{5/2}}{2\sqrt{5}}\,\|\alpha\|_\infty^2\|\nabla' w_0\| = \frac{\varepsilon^2}{2\sqrt{5}}\,\|\alpha\|_\infty^2\|\nabla' w_0\|_\varepsilon , \\ \|w_0\nabla(\mathrm{e}^{-\mathrm{i}\alpha x_d}-1+\mathrm{i}\alpha x_d)\|_\varepsilon &\leqslant \frac{\varepsilon^{3/2}}{\sqrt{3}}\,\|\alpha\|_\infty\sqrt{\|\alpha\|_\infty^2+\|\nabla'\alpha\|_\infty^2\,\varepsilon^2}\,\|w_0\| \\ &= \frac{\varepsilon}{\sqrt{3}}\,\|\alpha\|_\infty\sqrt{\|\alpha\|_\infty^2+\|\nabla'\alpha\|_\infty^2\,\varepsilon^2}\,\|w_0\|_\varepsilon ,\end{aligned}$$

and the Schwarz inequality, we may write

$$\|(\mathrm{e}^{-\mathrm{i}\alpha x_d}-1+\mathrm{i}\alpha x_d)w_0\|_{\varepsilon,1} \leqslant C_1(\varepsilon)\,\varepsilon\,\|w_0\|_{\varepsilon,1}$$

with the same constant $C_1(\varepsilon)$ as defined in Theorem 14.1. Consequently, using (14.18), Lemma 14.4, Lemma 14.3 and the Schwarz inequality employing (14.16), we get the bound

$$\|u-(1+Q)w_0\|_{\varepsilon,1} \leqslant C(\varepsilon)\,\varepsilon\,\|f\|_\varepsilon$$

with

$$C(\varepsilon) := \sqrt{\frac{1}{\pi^2}+\Big(C_0+C_1(\varepsilon)\Big)^2}\,. \tag{14.23}$$

Note that $C(\varepsilon)$ coincides with the corresponding constant of Theorem 14.1. This concludes the proof of Theorem 14.1.

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Chapter 15

Reduction of dimension as a consequence of norm-resolvent convergence and applications

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Reduction of dimension as a consequence of norm-resolvent convergence and applications

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Abstract. This paper is devoted to dimensional reductions via the norm resolvent convergence. We derive explicit bounds on the resolvent difference as well as spectral asymptotics. The efficiency of our abstract tool is demonstrated by its application on seemingly different PDE problems from various areas of mathematical physics; all are analysed in a unified manner now, known results are recovered and new ones established.

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Keywords: reduction of dimension, norm resolvent convergence, Born-Oppenheimer approximation, thin layers, quantum waveguides, effective Hamiltonian.

15.1 Introduction

15.1.1 Motivation and context

In this paper we develop an abstract tool for dimensional reductions via the norm resolvent convergence obtained from variational estimates. The results are relevant in particular for PDE problems, typically Schrödinger-type operators depending on an asymptotic parameter having various interpretations (semiclassical limit, shrinking limits, large coupling limit, etc.). In applications, our resolvent estimates lead to accurate spectral asymptotic results for eigenvalues lying in a suitable region of the complex plane. Moreover, avoiding the traditional min-max approach, with its fundamental limitations to self-adjoint cases, we obtain an effective operator, the spectrum of which determines the spectral asymptotics. The flexibility of the latter is illustrated on a non-self-adjoint example in the second part of the paper.

The power of our approach is demonstrated by a unified treatment of diverse classical as well as recent problems occurring in mathematical physics such as:

- semiclassical Born-Oppenheimer approximation,
- shrinking tubular neighborhoods of hypersurfaces subject to various boundary conditions,
- domains with very attractive Robin boundary conditions.

In spite of the variety of operators, asymptotic regimes, and techniques considered in the previous literature, all these results are covered in our general abstract and not only asymptotic setting. Our first result (Theorem 15.1) gives a norm resolvent convergence towards a tensorial operator in a general self-adjoint setting. We emphasize that only two quantities need to be controlled: the size of a commutator of a "longitudinal operator" with spectral projection on low lying "transverse modes" and the size of the "spectral gap" of a "transverse operator", see (15.5) and (15.2), respectively. Although the latter is also very natural it was hardly visible in existing literature due to many seemingly different technical steps as well as various ways how these quantities enter. As particular cases of the application of Theorem 15.1, we recover, in a short manner, known results for quantum waveguides (see for instance [3], [12], [10] or [11]) and cast a new light on Born-Oppenheimer type results (see [13], [19], [8] or [18, Sec. 6.2]). To keep the presentation short we deliberately do not strive for the weakest possible assumptions in examples, although the abstract setting allows for many further generalizations and it clearly indicates how to proceed. We also remark that for more specific geometric situations sharper spectral results can be obtained, for example leading to perturbation series to higher order (see the book [15] and the survey article [5]).

In the second part of the paper, we prove, in the same spirit as previous results, the norm convergence result for a non-self-adjoint Robin Laplacian, see Theorem 15.2. It will partially generalize previous works in the self-adjoint (see [17], [9] and [16]) and in the non-self-adjoint (see [2]) cases.

As a matter of fact, the crucial step in all the proofs of the paper is an abstract lemma (see Lemma 15.1) of an independent interest. It provides a norm resolvent estimate from variational estimates, which is particularly suitable for the analysis of operators defined via sesquilinear forms.

15.1.2 Reduction of dimension in an abstract setting and self-adjoint applications

We first describe the reduction of dimension for an operator of the form

$$\mathscr{L} = S^*S + T, \qquad T = \bigoplus_{s\in\Sigma} T_s, \tag{15.1}$$

acting on the Hilbert space $\mathcal{H} = \bigoplus_{s\in\Sigma}\mathcal{H}_s$. The norm and inner product in $\mathcal{H}$ will be denoted by $\|\cdot\|$ and $\langle\cdot,\cdot\rangle$, respectively; the latter is assumed to be linear in the second argument.

Here Σ is a measure space and T_s is a self-adjoint non-negative operator on a Hilbert space $\mathcal{H}_s$ for all $s \in \Sigma$. Precise definitions will be given in Section 15.2. A typical example is the Schrödinger operator

$$H = (-i\hbar\partial_s)^2 + (-i\partial_t)^2 + V(s,t)\,,$$

acting on $L^2(\mathbb{R}_s \times \mathbb{R}_t)$. Here $\Sigma = \mathbb{R}$, $\mathcal{H}_s = L^2(\mathbb{R})$, $S = -i\hbar\partial_s$ and $T_s = (-i\partial_t)^2 + V(s,t)$.

We consider a function $s \mapsto \gamma_s$ such that

$$\gamma = \inf_{s\in\Sigma}\gamma_s > 0\,. \tag{15.2}$$

Then we denote by $\Pi_s \in \mathcal{L}(\mathcal{H}_s)$ the spectral projection of T_s on $[0,\gamma_s)$, and we set $\Pi_s^\perp = \mathrm{Id}_{\mathcal{H}_s} - \Pi_s$. We denote by Π the bounded operator on $\mathcal{H}$ such that for $\Phi \in \mathcal{H}$ and $s \in \Sigma$ we have $(\Pi\Phi)_s = \Pi_s\Phi_s$. We similarly define $\Pi^\perp \in \mathcal{L}(\mathcal{H})$. Our purpose is to compare some spectral properties of the operator $\mathscr{L}$ with those of the simpler operator

$$\mathscr{L}_{\mathsf{eff}} = \Pi\mathscr{L}\Pi. \tag{15.3}$$

This is an operator on $\Pi\mathcal{H}$ with domain $\Pi\mathcal{H} \cap \mathsf{D}(\mathscr{L})$.

In fact, we will first compare $\mathscr{L}$ with

$$\widehat{\mathscr{L}} = \Pi\mathscr{L}\Pi + \Pi^\perp\mathscr{L}\Pi^\perp. \tag{15.4}$$

Then $\mathscr{L}_{\mathsf{eff}}$ and $\mathscr{L}^\perp$ will be defined as the restrictions of $\widehat{\mathscr{L}}$ to $\Pi\mathcal{H}$ and $\Pi^\perp\mathcal{H}$, respectively, so that

$$\widehat{\mathscr{L}} = \mathscr{L}_{\mathsf{eff}} \oplus \mathscr{L}^\perp.$$

We will give a sufficient condition for $z \in \rho(\widehat{\mathscr{L}})$ to be in $\rho(\mathscr{L})$ and, in this case, an estimate for the difference of the resolvents. Then, since $\Pi\mathcal{H}$ and $\Pi^\perp\mathcal{H}$ reduce $\widehat{\mathscr{L}}$, it is not difficult to check that far from the spectrum of $\mathscr{L}^\perp$ the spectral properties of $\widehat{\mathscr{L}}$ are the same as those of $\mathscr{L}_{\mathsf{eff}}$, so we can state a similar statement with $\widehat{\mathscr{L}}$ replaced by $\mathscr{L}_{\mathsf{eff}}$. In applications, we can for instance prove that the first eigenvalues of $\mathscr{L}$ are close to the eigenvalues of the simpler operator $\mathscr{L}_{\mathsf{eff}}$.

We assume that $\mathsf{D}(S)$ is invariant under Π, that $[S,\Pi]$ extends to a bounded operator on $\mathcal{H}$, and we set

$$a = \frac{\|[S,\Pi]\|_{\mathcal{L}(\mathcal{H})}}{\sqrt{\gamma}}\,. \tag{15.5}$$

For $z \in \mathbb{C}$, we also define

$$\begin{aligned}
\eta_1(z) &= \frac{3}{\sqrt{2}}a^2\gamma + \frac{6a}{\sqrt{2}}(1+a)|z| + \frac{3a}{\gamma\sqrt{2}}\left(2 + \frac{a}{\sqrt{2}}\right)|z|^2\,,\\
\eta_2(z) &= \frac{3a}{\sqrt{2}}(1+a) + \frac{3a}{\gamma\sqrt{2}}\left(2 + \frac{a}{\sqrt{2}}\right)|z|\,,\\
\eta_3(z) &= \frac{3a}{\sqrt{2}}\left(1 + \frac{a}{\sqrt{2}}\right) + \frac{3a}{\gamma\sqrt{2}}\left(2 + \frac{a}{\sqrt{2}}\right)|z|\,,\\
\eta_4(z) &= \frac{3a}{\gamma\sqrt{2}}\left(2 + \frac{a}{\sqrt{2}}\right)\,.
\end{aligned} \tag{15.6}$$

Here a and γ are respectively related to the aforementioned "size of commutator" and the "spectral gap", and z will play the role of a spectral parameter. Various applications of our main theorems will illustrate what the orders of magnitude of a and γ can be.

Theorem 15.1. *Let $z \in \rho(\widehat{\mathscr{L}})$. If*

$$1 - \eta_1(z)\|(\widehat{\mathscr{L}} - z)^{-1}\| - \eta_2(z) > 0,$$

then $z \in \rho(\mathscr{L})$ and

$$\begin{aligned}\|(\mathscr{L} - z)^{-1} - (\widehat{\mathscr{L}} - z)^{-1}\| \\ \leq \eta_1(z)\|(\mathscr{L} - z)^{-1}\|\|(\widehat{\mathscr{L}} - z)^{-1}\| + \eta_2(z)\|(\mathscr{L} - z)^{-1}\| + \eta_3(z)\|(\widehat{\mathscr{L}} - z)^{-1}\| + \eta_4(z).\end{aligned}$$

In particular,

$$\|(\mathscr{L} - z)^{-1}\| \leq \frac{(\eta_3(z)+1)\|(\widehat{\mathscr{L}} - z)^{-1}\| + \eta_4(z)}{1 - \eta_1(z)\|(\widehat{\mathscr{L}} - z)^{-1}\| - \eta_2(z)}.$$

In order to compare the resolvent of $\mathscr{L}$ to the resolvent of $\mathscr{L}_{\mathsf{eff}}$, this theorem is completed by the following easy estimate:

Proposition 15.1. *We have $\mathsf{Sp}(\widehat{\mathscr{L}}) = \mathsf{Sp}(\mathscr{L}_{\mathsf{eff}}) \cup \mathsf{Sp}(\mathscr{L}^{\perp})$ and, for $z \in \rho(\widehat{\mathscr{L}})$ such that $z \notin [\gamma, +\infty)$,*

$$\left\|(\widehat{\mathscr{L}} - z)^{-1} - (\mathscr{L}_{\mathsf{eff}} - z)^{-1}\Pi\right\| \leq \frac{1}{\mathsf{dist}(z, [\gamma, +\infty))}.$$

In this estimate, it is implicit that $(\mathscr{L}_{\mathsf{eff}} - z)^{-1}$ is composed on the left by the inclusion $\Pi\mathcal{H} \to \mathcal{H}$.

Remark 15.1. These results cover a wide range of situations. In Section 15.3, we will discuss three paradigmatic applications. The space Σ will be $\mathbb{R}$ or a submanifold of $\mathbb{R}^d$, $d \geq 2$. The set $\mathcal{H}_s$ is fixed, but the Hilbert structure thereon may depend on s. In our examples $(T_s)_{s\in\Sigma}$ is related to an analytic family of self-adjoint operators which are not necessarily non-negative. Nevertheless, under suitable assumptions, we can reduce ourselves to the non-negative case. Indeed, in our applications, we will consider a family $(\tilde{T}_s)_{s\in\Sigma}$ of operators bounded from below, independently of $s \in \Sigma$. Moreover, the bottom of the spectrum of $\tilde{T}_s$ will be an isolated simple eigenvalue $\tilde{\mu}_1(s)$. Then, we notice that $\inf_{s\in\Sigma} \tilde{\mu}_1(s)$ is well-defined and that $T_s = \tilde{T}_s - \inf_{s\in\Sigma} \tilde{\mu}_1(s)$ is non-negative. We denote by $u_1(s)$ a corresponding eigenfunction. We can assume that $\|u_1(s)\|_{\mathcal{H}} = 1$ for all $s \in \Sigma$ and that u_1 is a smooth function of s. Π_s is the projection on $u_1(s)$ and $\Pi\mathcal{H}$ can be identified with $L^2(\Sigma)$ via the map $\varphi \mapsto (s \mapsto \varphi(s)u_1(s))$. In particular $\mathscr{L}_{\mathsf{eff}}$ can be seen as an operator on $L^2(\Sigma)$, which is what is meant by the "reduction of dimension". Finally, γ_s is defined as the bottom $\tilde{\mu}_2(s) - \inf_{s\in\Sigma} \tilde{\mu}_1(s)$ of the remaining part of the spectrum and

$$\gamma = \inf_s \tilde{\mu}_2(s) - \inf_s \tilde{\mu}_1(s) \leq \inf \mathsf{Sp}((\mathscr{L} - \inf_{s\in\Sigma} \tilde{\mu}_1(s))^{\perp}). \tag{15.7}$$

We recall that we assume the spectral gap condition $\gamma > 0$, see (15.2).

15.1.3 The Robin Laplacian in a shrinking layer as a non-self-adjoint application

We now consider a reduction of dimension result in a non-self-adjoint setting, namely the Robin Laplacian in a shrinking layer. Let $d \geq 2$. Here, Σ is an orientable smooth (compact or non-compact) hypersurface in $\mathbb{R}^d$ without boundary. The orientation can be specified by a globally defined unit normal vector field $n : \Sigma \to \mathbb{S}^{d-1}$. Moreover Σ is endowed with the Riemannian structure inherited from the Euclidean structure defined on $\mathbb{R}^d$. We assume that Σ admits a tubular neighborhood, i.e. for $\varepsilon > 0$ small enough the map

$$\Theta_\varepsilon : (s, t) \mapsto s + \varepsilon t n(s) \tag{15.8}$$

is injective on $\overline{\Sigma} \times [-1, 1]$ and defines a diffeomorphism from $\Sigma \times (-1, 1)$ to its image. We set

$$\Omega = \Sigma \times (-1, 1) \quad \text{and} \quad \Omega_\varepsilon = \Theta_\varepsilon(\Omega). \tag{15.9}$$

Then Ω_ε has the geometrical meaning of a non-self-intersecting layer delimited by the hypersurfaces

$$\Sigma_{\pm,\varepsilon} = \Theta_\varepsilon(\Sigma \times \{\pm 1\}).$$

Moreover $\Sigma_{\pm,\varepsilon}$ can be identified with Σ via the diffeomorphisms

$$\Theta_{\pm,\varepsilon} : \begin{cases} \Sigma & \to & \Sigma_{\pm,\varepsilon} \\ s & \mapsto & s \pm \varepsilon n(s). \end{cases}$$

Let $\alpha : \Sigma \to \mathbb{C}$ be a smooth bounded function. We set $\alpha_{\pm,\varepsilon} = \alpha \circ \Theta_{\pm,\varepsilon}^{-1} : \Sigma_{\pm,\varepsilon} \to \mathbb{C}$ and we consider on $L^2(\Omega_\varepsilon)$ the closed operator $\mathscr{P}_{\varepsilon,\alpha}$ (or simply $\mathscr{P}_\varepsilon$ if no risk of confusion) defined as the usual Laplace operator on Ω_ε subject to the Robin boundary condition

$$\frac{\partial u}{\partial n} + \alpha_{\pm,\varepsilon} u = 0, \quad \text{on } \Sigma_{\pm,\varepsilon}. \tag{15.10}$$

Remark 15.2. Note that a very special choice of Robin boundary conditions is considered in this section. Indeed, the boundary-coupling functions considered on $\Sigma_{+,\varepsilon}$ and $\Sigma_{-,\varepsilon}$ are the same except for a switch of sign, see (15.25). More specifically, $\alpha_{\pm,\varepsilon}(s) = \alpha(s)$ for every $s \in \Sigma$ and n is an outward normal to Ω_ε on one of the connected parts $\Sigma_{\pm,\varepsilon}$ of the boundary $\partial\Omega_\varepsilon$, while it is inward pointing on the other boundary. This special choice is motivated by Parity-Time-symmetric waveguides [1, 2] as well as by a self-adjoint analogue considered in [16]. It is straightforward to extend the present procedure to the general situation of two different boundary-coupling functions on $\Sigma_{+,\varepsilon}$ and $\Sigma_{-,\varepsilon}$, but then the effective operator will be ε-dependent (in analogy with the Dirichlet boundary conditions, see Proposition 15.6) or a renormalization would be needed (cf. [12]).

Our purpose is to prove that, at the limit when ε goes to 0, the operator $\mathscr{P}_\varepsilon$ converges in a norm-resolvent sense to a Schrödinger operator

$$\mathscr{L}_{\mathsf{eff}} = -\Delta_\Sigma + V_{\mathsf{eff}}\,,$$

on Σ. Here $-\Delta_\Sigma$ is the Laplace-Beltrami operator on Σ, and the potential V_{eff} depends both on the geometry of Σ and on the boundary condition. More precisely we have

$$V_{\mathsf{eff}} = |\alpha|^2 - 2\alpha\Re(\alpha) - \alpha(\kappa_1 + \cdots + \kappa_{d-1}). \tag{15.11}$$

Note that the sum of the principal curvatures is proportional to the mean curvature of Σ.

It will appear later that the shrinking limit $\varepsilon \to 0$ strongly penalizes the normal derivative (independently of the boundary condition). Thus we consider $\Pi \in \mathcal{L}(L^2(\Omega))$ the projection on functions which do not depend on t: for $u \in L^2(\Omega)$ and $(s,t) \in \Omega$ we set

$$(\Pi u)(s,t) = \frac{1}{2}\int_{-1}^{1} u(s,\theta)\mathrm{d}\theta\,.$$

Then we define $\Pi^\perp = \mathrm{Id} - \Pi$.

Theorem 15.2. *Let K be a compact subset of $\rho(H^{\mathsf{eff}})$. Then there exists $\varepsilon_0 > 0$ and $C \geq 0$ such that for $z \in K$ and $\varepsilon \in (0,\varepsilon_0)$ we have $z \in \rho(H_\varepsilon)$ and*

$$\|(\mathscr{P}_\varepsilon - z)^{-1} - U_\varepsilon^{-1}(\mathscr{L}_{\mathsf{eff}} - z)^{-1}\Pi U_\varepsilon\|_{\mathcal{L}(L^2(\Omega_\varepsilon))} \leq C\varepsilon\,.$$

Here U_ε is a unitary transformation from $L^2(\Omega_\varepsilon, \mathrm{d}x)$ to $L^2(\Omega, w_\varepsilon(x)\mathrm{d}\sigma\mathrm{d}t)$, where for some $C > 1$ we have

$$\forall\varepsilon \in (0,\varepsilon_0), \forall x \in \Omega, \quad \frac{1}{C} \leq |w_\varepsilon(x)| \leq C\,.$$

As for Theorem 15.1 it is implicit that the resolvent $(\mathscr{L}_{\mathsf{eff}} - z)^{-1}$ is composed on the left by the inclusion $\Pi L^2(\Omega_\varepsilon) \to L^2(\Omega_\varepsilon)$. Moreover the operator $\mathscr{L}_{\mathsf{eff}}$ on $L^2(\Sigma)$ has been identified with an operator on $\Pi L^2(\Omega_\varepsilon)$.

Remark 15.3. In the geometrically trivial situation $\Sigma = \mathbb{R}^{d-1}$ and special choice $\Re(\alpha) = 0$, a version of Theorem 15.2 was previously established in [2]. At the same time, in the self-adjoint case $\Im(\alpha) = 0$ and very special geometric setting $d = 1$ (Σ being a curve), a version of Theorem 15.2 is due to [16]. In our general setting, it is interesting to see how the geometry enters the effective dynamics, through the mean curvature of Σ, see (15.11).

15.1.4 From variational estimates to norm resolvent convergence

All the results of this paper are about estimates of the difference of resolvents of two operators. These estimates will be deduced from the corresponding estimates of the associated quadratic forms by the following general lemma:

Lemma 15.1. *Let $\mathcal{K}$ be a Hilbert space. Let $\mathcal{A}$ and $\widehat{\mathcal{A}}$ be two closed densely defined operators on $\mathcal{K}$. Assume that $\widehat{\mathcal{A}}$ is bijective and that there exist $\eta_1, \eta_2, \eta_3, \eta_4 \geq 0$ such that $1 - \eta_1\|\widehat{\mathcal{A}}^{-1}\| - \eta_2 > 0$ and*

$$\forall\phi \in \mathsf{D}(\mathcal{A}), \forall\psi \in \mathsf{D}(\widehat{\mathcal{A}}^*)\,,$$
$$|\langle\mathcal{A}\phi,\psi\rangle - \langle\phi,\widehat{\mathcal{A}}^*\psi\rangle| \leq \eta_1\|\phi\|\|\psi\| + \eta_2\|\phi\|\|\widehat{\mathcal{A}}^*\psi\| + \eta_3\|\mathcal{A}\phi\|\|\psi\| + \eta_4\|\mathcal{A}\phi\|\|\widehat{\mathcal{A}}^*\psi\|\,.$$

Then $\mathcal{A}$ is injective with closed range. If moreover $\mathcal{A}^*$ is injective, then $\mathcal{A}$ is bijective and we have the estimates

$$\|\mathcal{A}^{-1}\| \leq \frac{(\eta_3+1)\|\hat{\mathcal{A}}^{-1}\| + \eta_4}{1 - \eta_1\|\widehat{\mathcal{A}}^{-1}\| - \eta_2} \tag{15.12}$$

and

$$\left\|\mathcal{A}^{-1} - \widehat{\mathcal{A}}^{-1}\right\| \leq \eta_1\|\mathcal{A}^{-1}\|\|\widehat{\mathcal{A}}^{-1}\| + \eta_2\|\mathcal{A}^{-1}\| + \eta_3\|\widehat{\mathcal{A}}^{-1}\| + \eta_4.$$

Since the proof is rather elementary, let us provide it already now.

Proof. Let $\phi \in \mathsf{D}(\mathcal{A})$ and consider $\psi = (\widehat{\mathcal{A}}^{-1})^*\phi \in \mathsf{D}(\widehat{\mathcal{A}}^*)$. We have

$$\begin{aligned}|\|\phi\|^2 - \langle \mathcal{A}\phi, (\widehat{\mathcal{A}}^{-1})^*\phi\rangle| &= |\langle \phi, \widehat{\mathcal{A}}^*\psi\rangle - \langle \mathcal{A}\phi, \psi\rangle| \\ &\leq (\eta_1\|\widehat{\mathcal{A}}^{-1}\| + \eta_2)\|\phi\|^2 + \left(\eta_3\|\widehat{\mathcal{A}}^{-1}\| + \eta_4\right)\|\mathcal{A}\phi\|\|\phi\|\,,\end{aligned}$$

so

$$\|\phi\|^2 \leq \left(\eta_1\|\hat{\mathcal{A}}^{-1}\| + \eta_2\right)\|\phi\|^2 + \left((\eta_3+1)\|\hat{\mathcal{A}}^{-1}\| + \eta_4\right)\|\phi\|\|\mathcal{A}\phi\|.$$

Then if $\eta_1\|\widehat{\mathcal{A}}^{-1}\| + \eta_2 < 1$, we get

$$\|\phi\| \leq \frac{(\eta_3+1)\|\hat{\mathcal{A}}^{-1}\| + \eta_4}{1 - \eta_1\|\widehat{\mathcal{A}}^{-1}\| - \eta_2}\|\mathcal{A}\phi\|\,. \tag{15.13}$$

In particular, $\mathcal{A}$ is injective with closed range. If $\mathcal{A}^*$ is injective, the range of $\mathcal{A}$ is dense and thus $\mathcal{A}$ is bijective. In particular, with (15.13), we obtain (15.12).

Finally for $f, g \in \mathcal{K}$, $\phi = \mathcal{A}^{-1}f$ and $\psi = (\widehat{\mathcal{A}}^{-1})^*g$ we have

$$\langle\left(\mathcal{A}^{-1} - \widehat{\mathcal{A}}^{-1}\right)f, g\rangle = \langle \phi, \widehat{\mathcal{A}}^*\psi\rangle - \langle \mathcal{A}\phi, \psi\rangle,$$

and the conclusion follows by easy manipulations. □

15.1.5 Organization of the paper

In Section 15.2, we prove Theorem 15.1. We first define the operators $\mathscr{L}$, $\widehat{\mathscr{L}}$ and $\mathscr{L}_{\mathsf{eff}}$, and then we show how Lemma 15.1 can be applied. In Section 15.3, we discuss some applications of Theorem 15.1 to the semiclassical Born-Oppenheimer approximation, the Dirichlet Laplacian on a shrinking tubular neighborhood of an hypersurface and the Robin Laplacian in the large coupling limit. Section 15.4 is devoted to the proof of Theorem 15.2 about the non-self-adjoint Robin Laplacian on a shrinking layer.

15.2 Abstract reduction of dimension

In this section we describe more precisely the setting introduced in Section 15.1.2 and we prove Theorem 15.1. The applications will be given in the following section.

15.2.1 Definition of the effective operator

Let (Σ, σ) be a measure space. For each $s \in \Sigma$ we consider a separable complex Hilbert space $\mathcal{H}_s$. Then, on $\mathcal{H}_s$ we consider a closed symmetric non-negative sesquilinear form q_s with dense domain $\mathsf{D}(q_s)$. We denote by T_s the corresponding self-adjoint and non-negative operator, as given by the Representation Theorem. As already said in Section 15.1.2, we consider a function $s \in \Sigma \mapsto \gamma_s \in \mathbb{R}$ whose infimum is positive, see (15.2). Then we denote by $\Pi_s \in \mathcal{L}(\mathcal{H}_s)$ the spectral projection of T_s on $[0, \gamma_s)$, and we set $\Pi_s^\perp = \mathrm{Id}_{\mathcal{H}_s} - \Pi_s$.

We denote by $\mathcal{H}$ the subset of $\bigoplus_{s\in\Sigma}\mathcal{H}_s$ which consists of all $\Phi = (\Phi_s)_{s\in\Sigma}$ such that the functions $s \mapsto \|\Phi_s\|_{\mathcal{H}_s}$ and $s \mapsto \|\Pi_s\Phi_s\|_{\mathcal{H}_s}$ are measurable on Σ and

$$\|\Phi\|^2 = \int_\Sigma \|\Phi_s\|^2_{\mathcal{H}_s}\mathrm{d}\sigma(s) < +\infty\,.$$

It is endowed with the Hilbert structure given by this norm. We denote by Π the bounded operator on $\mathcal{H}$ such that for $\Phi \in \mathcal{H}$ and $s \in \Sigma$ we have $(\Pi\Phi)_s = \Pi_s\Phi_s$. We similarly define $\Pi^\perp \in \mathcal{L}(\mathcal{H})$.

The forms q_s on $\mathcal{H}_s$ define a quadratic form Q_T on $\mathcal{H}$ as follows. We say that $\Phi = (\Phi_s)_{s\in\Sigma} \in \mathcal{H}$ belongs to $\mathsf{D}(Q_T)$ if Φ_s belongs to $\mathsf{D}(q_s)$ for all $s \in \Sigma$, the functions $s \mapsto q_s(\Phi_s)$ and $s \mapsto q_s(\Pi_s\Phi_s)$ are measurable on Σ and

$$Q_T(\Phi) = \int_\Sigma q_s(\Phi_s)\mathrm{d}\sigma(s) < +\infty\,.$$

We consider on $\mathcal{H}$ an operator S with dense domain $\mathsf{D}(S)$. We assume that $\mathsf{D}(S)$ is invariant under Π, that $[S, \Pi]$ extends to a bounded operator on $\mathcal{H}$, and we define a as in (15.5). We assume that

$$\mathsf{D}(Q) = \mathsf{D}(S) \cap \mathsf{D}(Q_T)$$

is dense in $\mathcal{H}$, and for $\Phi \in \mathsf{D}(Q)$ we set

$$Q(\Phi) = \|S\Phi\|^2 + Q_T(\Phi)\,. \tag{15.14}$$

We assume that Q defines a closed form on $\mathcal{H}$. The form Q is symmetric and non-negative and the associated operator is the operator $\mathscr{L}$ introduced in (15.1).

Then we define the operator $\widehat{\mathscr{L}}$ (see (15.4)) by its form. For this we need to verify that the form domain is left invariant both by Π and $\Pi^\perp$.

Lemma 15.2. *For all $\Phi \in \mathsf{D}(Q)$ we have $\Pi\Phi \in \mathsf{D}(Q)$ and $\Pi^\perp\Phi \in \mathsf{D}(Q)$.*

Proof. Let $\Phi = (\Phi_s)_{s\in\Sigma} \in \mathsf{D}(Q)$. We have $\Phi \in \mathsf{D}(S)$, so by assumption we have $\Pi\Phi \in \mathsf{D}(S)$. By assumption again, the function $s \mapsto q_s(\Pi_s\Phi_s) = q_s(\Pi_s\Pi_s\Phi_s)$ is measurable and we have

$$\int_\Sigma q_s(\Pi_s\Phi_s)\, d\sigma(s) \le \sup_{s\in\Sigma}\gamma_s \int_\Sigma \|\Phi_s\|^2_{\mathcal{H}_s}\, d\sigma(s) < +\infty.$$

This proves that $\Pi\Phi$ belongs to $\mathsf{D}(Q_T)$, and hence to $\mathsf{D}(Q)$. Then the same holds for $\Pi^\perp\Phi = \Phi - \Pi\Phi$. ☐

With this lemma we can set, for $\Phi, \Psi \in \mathsf{D}(Q)$,

$$\widehat{Q}(\Phi,\Psi) = Q(\Pi\Phi,\Pi\Psi) + Q(\Pi^\perp\Phi,\Pi^\perp\Psi)\,.$$

Lemma 15.3. *For all $\Phi \in \mathsf{D}(\widehat{Q})$ we have*

$$Q(\Phi) \le 2\widehat{Q}(\Phi)\,.$$

In particular the form $\widehat{Q}$ is non-negative, closed, and it determines uniquely a self-adjoint operator $\widehat{\mathscr{L}}$ on $\mathcal{H}$. Moreover we have $[\Pi, \widehat{\mathscr{L}}] = 0$ on $\mathsf{D}(\widehat{\mathscr{L}})$.

Proof. We have

$$Q(\Phi) - \widehat{Q}(\Phi) = Q(\Pi\Phi,\Pi^\perp\Phi) + Q(\Pi^\perp\Phi,\Pi\Phi)\,.$$

Since the form Q is non-negative we can apply the Cauchy-Schwarz inequality to write

$$Q(\Pi\Phi,\Pi^\perp\Phi) \le \sqrt{Q(\Pi\Phi)}\sqrt{Q(\Pi^\perp\Phi)} \le \frac{1}{2}\big(Q(\Pi\Phi) + Q(\Pi^\perp\Phi)\big) = \frac{1}{2}\widehat{Q}(\Phi)\,.$$

We have the same estimate for $Q(\Pi^\perp\Phi,\Pi\Phi)$, and the first conclusions follow. We just check the last property about the commutator. Let $\psi \in \mathsf{D}(\widehat{\mathscr{L}})$. For all $\phi \in \mathsf{D}(\widehat{\mathscr{L}})$ we have

$$\widehat{Q}(\phi,\Pi\psi) = Q(\Pi\phi,\Pi\psi) = \widehat{Q}(\Pi\phi,\psi) = \langle \Pi\phi, \widehat{\mathscr{L}}\psi\rangle_{\mathcal{H}} = \langle \phi, \Pi\widehat{\mathscr{L}}\psi\rangle_{\mathcal{H}}.$$

This proves that $\Pi\psi \in \mathsf{D}(\widehat{\mathscr{L}})$ with $\widehat{\mathscr{L}}\Pi\psi = \Pi\widehat{\mathscr{L}}\psi$ and the proof is complete. ☐

Then, from $\widehat{Q}$ it is easy to define the forms corresponding to the operators $\mathscr{L}_{\mathsf{eff}}$ and $\mathscr{L}^\perp$:

Lemma 15.4. *Let Q_{eff} be the restriction of Q to $\Pi\mathsf{D}(Q) = \mathrm{Ran}(\Pi) \cap \mathsf{D}(Q)$. Then Q_{eff} is non-negative and closed. The associated operator $\mathscr{L}_{\mathsf{eff}}$ is self-adjoint, its domain is invariant under Π, and $[\Pi, \mathscr{L}_{\mathsf{eff}}] = 0$ on $\mathsf{D}(\mathscr{L}_{\mathsf{eff}})$. Moreover, we have $(\mathsf{D}(\widehat{\mathscr{L}}) \cap \mathrm{Ran}(\Pi), \widehat{\mathscr{L}}) = (\mathsf{D}(\mathscr{L}_{\mathsf{eff}}), \mathscr{L}_{\mathsf{eff}})$.*

We have similar statements for the restriction $Q_\perp$ of Q to $\Pi^\perp\mathsf{D}(Q) = \mathrm{Ran}(\Pi^\perp)\cap\mathsf{D}(Q)$ and the corresponding operator $\mathscr{L}^\perp$.

Proof. The closedness of Q_{eff} comes from the closedness of Q and the continuity of Π. The other properties are proved as for Lemma 15.3. We prove the last assertion. Let $\psi \in \mathsf{D}(\mathscr{L}_{\mathsf{eff}})$. By definition of this domain we have $\Pi\psi = \psi$. For $\phi \in \mathsf{D}(\widehat{Q})$, we have

$$\widehat{Q}(\phi,\psi) = Q(\Pi\phi,\Pi\psi) = Q_{\mathsf{eff}}(\Pi\phi,\Pi\psi) = Q_{\mathsf{eff}}(\Pi\phi,\psi) = \langle \Pi\phi, \mathscr{L}_{\mathsf{eff}}\psi\rangle = \langle \phi, \mathscr{L}_{\mathsf{eff}}\psi\rangle\,.$$

This proves that $\psi \in \mathsf{D}(\widehat{\mathscr{L}})$ and $\mathscr{L}_{\mathsf{eff}}\psi = \widehat{\mathscr{L}}\psi$. Thus $\mathsf{D}(\mathscr{L}_{\mathsf{eff}}) \subset \mathsf{D}(\widehat{\mathscr{L}}) \cap \mathrm{Ran}(\Pi)$ and $\widehat{\mathscr{L}} = \mathscr{L}_{\mathsf{eff}}$ on $\mathsf{D}(\mathscr{L}_{\mathsf{eff}})$. The reverse inclusion $\mathsf{D}(\widehat{\mathscr{L}}) \cap \mathrm{Ran}(\Pi) \subset \mathsf{D}(\mathscr{L}_{\mathsf{eff}})$ is easy, so the proof is complete. ☐

Finally we have proved that

$$\mathsf{D}(\widehat{\mathscr{L}}) = \big(\mathsf{D}(\widehat{\mathscr{L}}) \cap \mathrm{Ran}(\Pi)\big) \oplus \big(\mathsf{D}(\widehat{\mathscr{L}}) \cap \mathrm{Ran}(\Pi^\perp)\big) = \mathsf{D}(\mathscr{L}_{\mathsf{eff}}) \oplus \mathsf{D}(\mathscr{L}^\perp)$$

and for $\varphi \in \mathsf{D}(\widehat{\mathscr{L}})$ we have

$$\widehat{\mathscr{L}}\varphi = \mathscr{L}_{\mathsf{eff}}\Pi\varphi + \mathscr{L}^\perp\Pi^\perp\varphi.$$

From the spectral theorem and $\mathsf{Sp}(\mathscr{L}^\perp) \subset [\gamma, +\infty)$, we deduce the following lemma.

Lemma 15.5. *We have $\mathsf{Sp}(\widehat{\mathscr{L}}) = \mathsf{Sp}(\mathscr{L}_{\mathsf{eff}}) \cup \mathsf{Sp}(\mathscr{L}^\perp)$ and, for $z \in \rho(\widehat{\mathscr{L}})$ such that $z \notin [\gamma, +\infty)$,*

$$\left\|(\widehat{\mathscr{L}} - z)^{-1} - (\mathscr{L}_{\mathsf{eff}} - z)^{-1}\Pi\right\| \le \frac{1}{\mathsf{dist}(z, [\gamma, +\infty))}\,.$$

15.2.2 Comparison of the resolvents

This section is devoted to the proof of the following theorem that implies Theorem 15.1 via Lemma 15.1.

Theorem 15.3. *Let $\mathscr{L}$ and $\widehat{\mathscr{L}}$ be as above. Let $z \in \mathbb{C}$ and $\eta_1(z), \eta_2(z), \eta_3(z), \eta_4(z)$ as in (15.6). Then for $\Phi \in \mathsf{D}(\mathscr{L})$ and $\Psi \in \mathsf{D}(\widehat{\mathscr{L}^*})$ we have*

$$|Q(\Phi,\Psi) - \widehat{Q}(\Phi,\Psi)| \leq \eta_1(z)\,\|\Phi\|\,\|\Psi\| + \eta_2(z)\|\Phi\|\|(\widehat{\mathscr{L}} - \bar{z})\Psi\| \\ + \eta_3(z)\|(\mathscr{L} - z)\Phi\|\|\Psi\| + \eta_4(z)\|(\mathscr{L} - z)\Phi\|\|(\widehat{\mathscr{L}} - \bar{z})\Psi\|\,.$$

Theorem 15.3 is a consequence of the following proposition after inserting z and using the triangular inequality.

Proposition 15.2. *For all $\Phi \in \mathsf{D}(\mathscr{L})$ and $\Psi \in \mathsf{D}(\widehat{\mathscr{L}})$ we have*

$$\frac{1}{\gamma}|Q(\Phi,\Psi) - \widehat{Q}(\Phi,\Psi)| \\ \leq \frac{3a}{\sqrt{2}}\left(\|\Phi\| + \frac{\|\mathscr{L}\Phi\|}{\gamma}\right)\frac{\|\widehat{\mathscr{L}}\Psi\|}{\gamma} + \frac{3a}{\sqrt{2}}\left(a\|\Phi\| + \left(1 + \frac{a}{\sqrt{2}}\right)\frac{\|\mathscr{L}\Phi\|}{\gamma}\right)\left(\|\Psi\| + \frac{\|\widehat{\mathscr{L}}\Psi\|}{\gamma}\right).$$

Proof. Let $\nu = \|[S,\Pi]\|$. We have

$$Q(\Phi,\Psi) - \widehat{Q}(\Phi,\Psi) = Q(\Pi^\perp\Phi, \Pi\Psi) + Q(\Pi\Phi, \Pi^\perp\Psi)\,.$$

For the first term we write

$$Q(\Pi^\perp\Phi, \Pi\Psi) = \langle S\Pi^\perp\Phi, S\Pi\Psi\rangle = \langle S\Pi^\perp\Phi, [S,\Pi]\Pi\Psi\rangle + \langle S\Pi^\perp\Phi, \Pi S\Pi\Psi\rangle\,,$$

so that

$$Q(\Pi^\perp\Phi, \Pi\Psi) = \langle S\Pi^\perp\Phi, [S,\Pi]\Pi\Psi\rangle + \langle [S,\Pi^\perp]\Pi^\perp\Phi, \Pi S\Pi\Psi\rangle\,.$$

We deduce that

$$|Q(\Pi^\perp\Phi, \Pi\Psi)| \leq \nu\|S\Pi^\perp\Phi\|\|\Psi\| + \nu\|\Pi^\perp\Phi\|\|S\Pi\Psi\|\,. \tag{15.15}$$

Similarly, we get, by slightly breaking the symmetry,

$$|Q(\Pi\Phi, \Pi^\perp\Psi)| \leq \nu\|S\Pi^\perp\Psi\|\|\Phi\| + \nu\|\Pi^\perp\Psi\|\|S\Phi\|\,. \tag{15.16}$$

We infer that

$$|Q(\Phi,\Psi) - \widehat{Q}(\Phi,\Psi)| \leq \nu\|S\Pi^\perp\Phi\|\|\Psi\| + \nu\|\Pi^\perp\Phi\|\|S\Pi\Psi\| + \nu\|S\Pi^\perp\Psi\|\|\Phi\| + \nu\|\Pi^\perp\Psi\|\|S\Phi\|\,. \tag{15.17}$$

Since Q_T is non-negative we have

$$\|S\Phi\|^2 \leq Q(\Phi) \leq \|\mathscr{L}\Phi\|\|\Phi\|. \tag{15.18}$$

Similarly,

$$\|S\Pi\Psi\|^2 \leq \widehat{Q}(\Psi) \leq \|\widehat{\mathscr{L}}\Psi\|\|\Psi\|\,. \tag{15.19}$$

Then we estimate $\|\Pi^\perp\Phi\|$ and $\|S\Pi^\perp\Phi\|$. We have

$$\langle \Pi^\perp\Phi, \mathscr{L}\Phi\rangle = Q(\Pi^\perp\Phi, \Phi) = Q(\Pi^\perp\Phi) + Q(\Pi^\perp\Phi, \Pi\Phi)\,,$$

and deduce

$$Q(\Pi^\perp\Phi) \leq \|\mathscr{L}\Phi\|\|\Pi^\perp\Phi\| + |Q(\Pi^\perp\Phi, \Pi\Phi)|\,.$$

From (15.16), we get

$$Q(\Pi^\perp\Phi) \leq \|\mathscr{L}\Phi\|\|\Pi^\perp\Phi\| + \nu\|S\Pi^\perp\Phi\|\|\Phi\| + \nu\|\Pi^\perp\Phi\|\|S\Phi\|\,.$$

Moreover, we have

$$Q(\Pi^\perp\Phi) \geq \|S\Pi^\perp\Phi\|^2 + \gamma\|\Pi^\perp\Phi\|^2\,.$$

We infer that

$$\|S\Pi^\perp\Phi\|^2 + \gamma\|\Pi^\perp\Phi\|^2 \\ \leq \frac{\gamma}{4}\|\Pi^\perp\Phi\|^2 + \frac{1}{\gamma}\|\mathscr{L}\Phi\|^2 + \frac{1}{2}\|S\Pi^\perp\Phi\|^2 + \frac{\nu^2}{2}\|\Phi\|^2 + \frac{\gamma}{4}\|\Pi^\perp\Phi\|^2 + \frac{\nu^2}{\gamma}\|S\Phi\|^2\,.$$

Using (15.18) we deduce that

$$\frac{1}{2}\left(\|S\Pi^{\perp}\Phi\|^2+\gamma\|\Pi^{\perp}\Phi\|^2\right)\leq\frac{1}{\gamma}\|\mathscr{L}\Phi\|^2+\frac{\nu^2}{2}\|\Phi\|^2+\frac{\nu^2}{2}\left(\frac{\|\mathscr{L}\Phi\|^2}{\gamma^2}+\|\Phi\|^2\right),$$

and thus

$$\frac{\|S\Pi^{\perp}\Phi\|^2}{\gamma}+\|\Pi^{\perp}\Phi\|^2\leq(2+a^2)\frac{\|\mathscr{L}\Phi\|^2}{\gamma^2}+2a^2\|\Phi\|^2\,. \tag{15.20}$$

Let us now consider $\|\Pi^{\perp}\Psi\|$ and $\|S\Pi^{\perp}\Psi\|$. We have easily that

$$\|S\Pi^{\perp}\Psi\|^2+\gamma\|\Pi^{\perp}\Psi\|^2\leq Q(\Pi^{\perp}\Psi)=\widehat{Q}(\Psi,\Pi^{\perp}\Psi)\leq\|\widehat{\mathscr{L}}\Psi\|\|\Pi^{\perp}\Psi\|\,,$$

and thus

$$\frac{\|S\Pi^{\perp}\Psi\|^2}{\gamma}+\|\Pi^{\perp}\Psi\|^2\leq\frac{\|\widehat{\mathscr{L}}\Psi\|^2}{\gamma^2}. \tag{15.21}$$

It remains to combine (15.17), (15.18), (15.19), (15.20), (15.21), and use elementary manipulations. □

15.3 Examples of applications

In this section we discuss three applications of Theorem 15.1 and we recall that we are in the context of Remark 15.1.

15.3.1 Semiclassical Born-Oppenheimer approximation

In this first example we set $(\Sigma,\sigma)=(\mathbb{R},\mathrm{d}s)$. We consider a Hilbert space $\mathcal{H}_T$ and set $\mathcal{H}=L^2(\mathbb{R},\mathcal{H}_T)$. Then, for $h>0$, we consider on $\mathcal{H}$ the operator $S_h=hD_s$, where $D_s=-i\partial_s$. We also consider an operator T on $\mathcal{H}$ such that for $\Phi=(\Phi_s)_{s\in\mathbb{R}}\in\mathcal{H}$ we have $(T\Phi)_s=T_s\Phi_s$, where (T_s) is a family of operators on the family of Hilbert spaces $(\mathcal{H}_s)$ which depends analytically on s. Thus the operator $\mathscr{L}=\mathscr{L}_h$ takes the form

$$\mathscr{L}_h=h^2D_s^2+T\,.$$

This kind of operators appears in [13, 14] where their spectral and dynamical behaviors are analyzed. As an example of operator T, the reader can have the Schrödinger operator $-\Delta_t+V(s,t)$ in mind, where the electric potential V is assumed to be real-valued. Here the operator norm of the commutator $[hD_s,\Pi]$ is controlled by h times the supremum of $\|\partial_s u_1(s)\|_{\mathcal{H}}$. Assuming that $\|\partial_s u_1(s)\|_{\mathcal{H}}$ is bounded, we have $a=a(h)=\mathcal{O}(h)$ (see (15.5)). Let us also assume, for our convenience, that μ_1 has a unique minimum, non-degenerate and not attained at infinity. Without loss of generality we can assume that this minimum is 0 and is attained at 0. Thus, here γ just satisfies $\gamma=\inf_{s\in\mathbb{R}}\mu_2(s)>0$.

For $k\in\mathbb{N}^*$ we set

$$\lambda_k(h)=\sup_{\substack{F\subset\mathsf{D}(\mathscr{L}_h)\\ \operatorname{codim}(F)=k-1}}\ \inf_{\substack{\varphi\in F\\ \|\varphi\|=1}}\langle\mathscr{L}_h\varphi,\varphi\rangle\,. \tag{15.22}$$

By the min-max principle, the first values of $\lambda_k(h)$ are given by the non-decreasing sequence of isolated eigenvalues of $\mathscr{L}_h$ (counted with multiplicities) below the essential spectrum. If there is a finite number of such eigenvalues, the rest of the sequence is given by the minimum of the essential spectrum. We similarly define the sequence $(\lambda_{\mathsf{eff},k}(h))$ corresponding to the operator $\mathscr{L}_{h,\mathsf{eff}}$. Note that $\mathscr{L}_{h,\mathsf{eff}}$ can be identified with the operator

$$h^2D_s^2+\mu_1(s)+h^2\|\partial_s u_1(s)\|^2_{\mathcal{H}_T}\,.$$

As a consequence of the harmonic approximation (see for instance [4, Chapter 7] or [18, Section 4.3.1]), we get the following asymptotics.

Proposition 15.3. *Let $k\in\mathbb{N}^*$. We have*

$$\lambda_{\mathsf{eff},k}(h)=(2k-1)\sqrt{\frac{\mu_1''(0)}{2}}h+o(h)\,,\qquad h\to 0\,.$$

From our abstract analysis, we deduce the following result.

Proposition 15.4. *Let $c_0,C_0>0$. There exist $h_0>0$ and $C>0$ such that for $h\in(0,h_0)$ and*

$$z\in\mathcal{Z}_h=\{z\in[-C_0h,C_0h]\,:\,\mathsf{dist}(z,\mathsf{Sp}(\mathscr{L}_{h,\mathsf{eff}}))\geq c_0h\}$$

we have $z\in\rho(\mathscr{L}_h)$ and

$$\|(\mathscr{L}_h-z)^{-1}-(\mathscr{L}_{h,\mathsf{eff}}-z)^{-1}\|\leq C\,.$$

Proof. Let $h > 0$ and $z \in \mathcal{Z}_h$. If h is small enough we have $C_0 h < \gamma$ so $z \in \rho(\mathscr{L}_{h,\mathsf{eff}}) \cap \rho(\mathscr{L}_h^\perp) = \rho(\widehat{\mathscr{L}_h})$. Moreover, by the Spectral Theorem,

$$\left\|(\widehat{\mathscr{L}_h} - z)^{-1}\right\| \leq \left\|(\mathscr{L}_{h,\mathsf{eff}} - z)^{-1}\right\| + \left\|(\mathscr{L}_h^\perp - z)^{-1}\right\| \leq \frac{1}{c_0 h} + \frac{1}{\gamma - C_0 h}.$$

With the notation (15.6) we have

$$\liminf_{h\to 0} \sup_{z\in Z_h} \Big(1 - \eta_{1,h}(z)\|(\widehat{\mathscr{L}_h} - z)^{-1}\| - \eta_{2,h}(z)\Big) > 0.$$

From Theorems 15.1 and Proposition 15.1, we deduce that $z \in \rho(\mathscr{L}_h)$,

$$\|(\mathscr{L}_h - z)^{-1}\| \lesssim h^{-1}\,,$$

and the estimate on the difference of the resolvents. Here and occasionally in the sequel, we adopt the notation $x \lesssim y$ if there is a positive constant C (independent of x and y) such that $x \leq Cy$. □

From this norm resolvent convergence result, we recover a result of [14, Section 4.2].

Proposition 15.5. *Let $k \in \mathbb{N}^*$. Then*

$$\lambda_k(h) = \lambda_{\mathsf{eff},k}(h) + \mathcal{O}(h^2), \quad h \to 0.$$

Proof. Let $\varepsilon > 0$ be such that $\lambda_{\mathsf{eff},k+1}(h) - \lambda_{\mathsf{eff},k}(h) > 2\varepsilon h$ for all h. We set $z_h = \lambda_{\mathsf{eff},k}(h) + \varepsilon h$. The resolvent $(\mathscr{L}_{h,\mathsf{eff}} - z_h)^{-1}$ has k negative eigenvalues

$$\frac{1}{\lambda_{\mathsf{eff},k}(h) - z_h} \leq \cdots \leq \frac{1}{\lambda_{\mathsf{eff},1}(h) - z_h},$$

all smaller than $-\alpha/h$ for some $\alpha > 0$, and the rest of the spectrum is positive. By Proposition 15.4 the resolvent $(\mathscr{L}_h - z_h)^{-1}$ is well defined for h small enough and there exists $C > 0$ such that

$$\left\|(\mathscr{L}_h - z_h)^{-1} - (\mathscr{L}_{h,\mathsf{eff}} - z_h)^{-1}\right\| \leq C.$$

By the min-max principle applied to these two resolvents, we obtain that for all $j \in \{1, \ldots, k\}$ the j-th eigenvalue of $(\mathscr{L}_h - z_h)^{-1}$ is at distance not greater than C from $1/(\lambda_{\mathsf{eff},k+1-j} - z_h)$, and the rest of the spectrum is greater than $-C$. In particular, for $j = 1$,

$$\left|\frac{1}{\lambda_k(h) - z_h} - \frac{1}{\lambda_{\mathsf{eff},k}(h) - z_h}\right| \leq C$$

so that

$$|\lambda_k(h) - \lambda_{\mathsf{eff},k}(h)| \leq C|\lambda_{\mathsf{eff},k}(h) - z_h||\lambda_k(h) - z_h|.$$

This gives

$$|\lambda_k(h) - \lambda_{\mathsf{eff},k}(h)| \leq C\varepsilon h|\lambda_k(h) - \lambda_{\mathsf{eff},k}(h) - \varepsilon h|,$$

and the conclusion follows for h small enough. □

15.3.2 Shrinking neighborhoods of hypersurfaces

In this paragraph we consider a submanifold Σ of $\mathbb{R}^d$, $d \geq 2$, as in Section 15.1.3. We choose $\varepsilon > 0$ and define Θ_ε, Ω and Ω_ε as in (15.8) and (15.9). For $\varphi \in H_0^1(\Omega_\varepsilon)$, we set

$$Q^{\mathsf{Dir}}_{\Omega_\varepsilon}(\varphi) = \int_{\Omega_\varepsilon} |\nabla\varphi|^2 \mathrm{d}x,$$

and we denote by $-\Delta^{\mathsf{Dir}}_{\Omega_\varepsilon}$ the associated operator. Then we use the diffeomorphism Θ_ε to see $-\Delta^{\mathsf{Dir}}_{\Omega_\varepsilon}$ as an operator on $L^2(\Omega)$. We set, for $\psi \in H_0^1(\Omega, \mathrm{d}\sigma\mathrm{d}t)$,

$$\mathcal{Q}^{\mathsf{Dir}}_\varepsilon(\psi) = Q^{\mathsf{Dir}}_{\Omega_\varepsilon}(\psi \circ \Theta_\varepsilon^{-1})\,.$$

We need a more explicit expression of $\mathcal{Q}^{\mathsf{Dir}}_\varepsilon$ in terms of the variables (s,t) on Ω. For $(s,t) \in \Omega$ we have on $T_{(s,t)}\Omega \simeq T_s\Sigma \times n(s)\mathbb{R}$

$$d_{(s,t)}\Theta_\varepsilon = (\mathsf{Id}_{T_s\Sigma} + \varepsilon t d_s n) \otimes \varepsilon \mathsf{Id}_{n(s)\mathbb{R}}\,.$$

Hence

$$d_{\Theta_\varepsilon(s,t)}\Theta_\varepsilon^{-1} = (\mathsf{Id}_{T_s\Sigma} + \varepsilon t d_s n)^{-1} \otimes \varepsilon^{-1}\mathsf{Id}_{n(s)\mathbb{R}}\,.$$

We recall that the Weingarten map $-d_s n$ is a self-adjoint operator on $T_s\Sigma$ (endowed with the metric inherited from the Euclidean structure on $\mathbb{R}^d$). For $\psi \in H^1(\Omega, \mathrm{d}\sigma\mathrm{d}t)$, $x \in \Omega_\varepsilon$ and $(s,t) = \Theta_\varepsilon^{-1}(x)$ we get

$$\begin{aligned}\|\nabla(\psi\circ\Theta_\varepsilon^{-1})(x)\|^2_{T_x\Omega_\varepsilon} &= \|(d_x\Theta_\varepsilon^{-1})^*\nabla\psi(s,t)\|^2_{T_x\Omega_\varepsilon}\\ &= \|(\mathsf{Id}_{T_s\Sigma} + \varepsilon t d_s n)^{-1}\nabla_s\psi(s,t)\|^2_{T_s\Sigma} + \frac{1}{\varepsilon^2}|\partial_t\psi(s,t)|^2\,.\end{aligned}$$

The eigenvalues of the Weingarten map are the principal curvatures $\kappa_1, \ldots, \kappa_{d-1}$. In particular for $(s,t) \in \Omega$ we have

$$\det(d_{(s,t)}\Theta_\varepsilon) = \varepsilon w_\varepsilon, \quad \text{where } w_\varepsilon(s,t) = \prod_{j=1}^{d-1}(1-\varepsilon t\kappa_j(s))\,. \tag{15.23}$$

The Riemannian structure on Ω is given by the pullback by Θ_ε of the Euclidean structure defined on Ω_ε. More explicitly, for $(s,t) \in \Omega$ the inner product on $T_{(s,t)}\Omega$ is given by

$$\forall X, Y \in T_{(s,t)}(\Omega), \quad g_\varepsilon(X,Y) = \langle d_{(s,t)}\Theta_\varepsilon(X), d_{(s,t)}\Theta_\varepsilon(Y)\rangle_{\mathbb{R}^d}\,.$$

Then the measure corresponding to the metric g_ε is given by $\varepsilon w_\varepsilon \mathrm{d}\sigma\mathrm{d}t$. Thus, if we set

$$G_\varepsilon(s,t) = (\mathsf{Id}_{T_s\Sigma} + \varepsilon t d_s n)^{-2}, \tag{15.24}$$

we finally obtain

$$\begin{aligned}\mathcal{Q}_\varepsilon^{\mathsf{Dir}}(\psi) &= \int_{\Omega_\varepsilon} |(\mathsf{Id}_{T_s\Sigma} + \varepsilon t d_s n)^{-1}\nabla_s\psi(\Theta_\varepsilon^{-1}(x))|^2\mathrm{d}x + \frac{1}{\varepsilon^2}\int_{\Omega_\varepsilon}|\partial_t\psi(\Theta_\varepsilon^{-1}(x))|^2\mathrm{d}x\\ &= \varepsilon\int_\Omega\langle G_\varepsilon(s,t)\nabla_s\psi, \nabla_s\psi\rangle_{T\Sigma}w_\varepsilon\mathrm{d}\sigma\mathrm{d}t + \frac{1}{\varepsilon^2}\int_\Omega|\partial_t\psi|^2\varepsilon w_\varepsilon\mathrm{d}\sigma\mathrm{d}t\,.\end{aligned}$$

The transverse operator $T_s(\varepsilon)$ is the Dirichlet realization on $L^2((-1,1), \varepsilon w_\varepsilon \mathrm{d}t)$ of the differential operator $-\varepsilon^{-2}w_\varepsilon^{-1}\partial_t w_\varepsilon\partial_t$. We denote by $\mu_1(s,\varepsilon)$ its first eigenvalue and we set $\mu(\varepsilon) = \inf_{s\in\Sigma}\mu_1(s,\varepsilon)$. We have, by perturbation theory, as $\varepsilon \to 0$,

$$\mu_1(s,\varepsilon) = \frac{\pi^2}{4\varepsilon^2} + V(s) + \mathcal{O}(\varepsilon)\,, \quad \mu(\varepsilon) = \frac{\pi^2}{4\varepsilon^2} + \mathcal{O}(1),$$

where the potential

$$V(s) = -\frac{1}{2}\sum_{j=1}^{d-1}\kappa_j(s)^2 + \frac{1}{4}\left(\sum_{j=1}^{d-1}\kappa_j(s)\right)^2$$

is assumed to be bounded from below.

We denote by $\mathscr{L}_\varepsilon^{\mathsf{Dir}}$ the operator associated to the form $\mathcal{Q}_\varepsilon^{\mathsf{Dir}}$ and by $\mathscr{L}_{\varepsilon,\mathsf{eff}}^{\mathsf{Dir}}$ the corresponding effective operator as defined in the general context of Section 15.1.2. It is nothing but the operator associated with the form $H^1(\Sigma) \ni \varphi \mapsto \mathcal{Q}_\varepsilon^{\mathsf{Dir}}(\varphi u_{s,\varepsilon})$ where $u_{s,\varepsilon}$ is the positive L^2-normalized groundstate of the transverse operator (and actually depending on the principal curvatures analytically). From perturbation theory, we can easily check that the commutator between the projection on $u_{s,\varepsilon}$ and $S = -iG_\varepsilon^{1/2}\nabla_s$ is bounded (and of order ε).

Proposition 15.6. *Let $c_0, C_0 > 0$. There exist $\varepsilon_0 > 0$ and $C > 0$ such that for all $\varepsilon \in (0,\varepsilon_0)$ and*

$$z \in \mathcal{Z}_{c_0,C_0,\varepsilon} = \{z \in \mathbb{R} : |z - \mu(\varepsilon)| \leq C_0\,, \quad \mathsf{dist}(z, \mathsf{Sp}(\mathscr{L}_{\varepsilon,\mathsf{eff}}^{\mathsf{Dir}})) \geq c_0\}$$

we have

$$\left\|\left(\mathscr{L}_\varepsilon^{\mathsf{Dir}} - z\right)^{-1} - \left(\mathscr{L}_{\varepsilon,\mathsf{eff}}^{\mathsf{Dir}} - z\right)^{-1}\right\| \leq C\varepsilon\,.$$

We recover a result of [11] (when there is no magnetic field).

Proof. We are in the context of Remark 15.1. The form $\mathcal{Q}_\varepsilon - \mu(\varepsilon)$ is non-negative. We denote by $\mathscr{L}_\varepsilon$ the corresponding non-negative self-adjoint operator and define $\widehat{\mathscr{L}_\varepsilon}$ as in Lemma 15.3. Given $\varepsilon > 0$ and $z \in \mathcal{Z}_{c_0,C_0,\varepsilon}$ we write ζ for $z - \mu(\varepsilon)$. Thus, with the notation of the abstract setting we have $\gamma_\varepsilon \sim \varepsilon^{-2}$, $a_\varepsilon = \mathcal{O}(\varepsilon^2)$, $\zeta = \mathcal{O}(1)$

and hence $\eta_{1,\varepsilon}(\zeta) = \mathcal{O}(\varepsilon)$, $\eta_{2,\varepsilon}(\zeta) = \mathcal{O}(\varepsilon^2)$, $\eta_{3,\varepsilon}(\zeta) = \mathcal{O}(\varepsilon)$ and $\eta_{4,\varepsilon}(\zeta) = \mathcal{O}(\varepsilon^2)$. Moreover, by the spectral theorem, we have

$$\left\| \left(\widehat{\mathscr{L}_\varepsilon} - \zeta\right)^{-1} \right\| = \mathcal{O}(1).$$

Thus, there exists $\varepsilon_0 > 0$ such that for $\varepsilon \in (0, \varepsilon_0)$, $z \in Z_{c_0,C_0,\varepsilon}$ and $\zeta = z - \mu(\varepsilon)$ the operator $\mathscr{L}_\varepsilon - \zeta$ is bijective and

$$\left\| (\mathscr{L}_\varepsilon - \zeta)^{-1} \right\| = \mathcal{O}(1)\,,$$

$$\left\| (\mathscr{L}_\varepsilon - \zeta)^{-1} - \left(\widehat{\mathscr{L}_\varepsilon} - \zeta\right)^{-1} \right\| = \mathcal{O}(\varepsilon)\,.$$

The conclusion easily follows. ☐

Given $\varepsilon > 0$ we define the sequence $(\lambda_k^{\mathsf{Dir}}(\varepsilon))_{k\in\mathbb{N}^*}$ and $(\lambda_{k,\mathsf{eff}}^{\mathsf{Dir}}(\varepsilon))_{k\in\mathbb{N}^*}$ corresponding to the operators $\mathscr{L}_\varepsilon^{\mathsf{Dir}}$ and $\mathscr{L}_{\varepsilon,\mathsf{eff}}^{\mathsf{Dir}}$ as in (15.22). By using analytic perturbation theory with respect to the parameters $(\varepsilon\kappa_j)_{1\leq j\leq d-1}$ to treat the commutator, we have, for all $k \in \mathbb{N}^*$,

$$\lambda_{k,\mathsf{eff}}^{\mathsf{Dir}}(\varepsilon) = \frac{\pi^2}{4\varepsilon^2} + \lambda_k^{\Sigma} + \mathcal{O}(\varepsilon)\,, \quad \varepsilon \to 0,$$

where λ_k^{Σ} is the k-th eigenvalue of $-\Delta_s + V(s)$.

We recover a result in the spirit of [3, 11].

Proposition 15.7. *For all $k \geq 1$ we have*

$$\lambda_k^{\mathsf{Dir}}(\varepsilon) = \frac{\pi^2}{4\varepsilon^2} + \lambda_k^{\Sigma} + \mathcal{O}(\varepsilon), \quad \varepsilon \to 0$$

Proof. Let $k \geq 1$. There exist $c_0, \tilde{c}_0, C_0, \varepsilon_0 > 0$ such that for $\varepsilon \in (0, \varepsilon_0)$ we have

$$\lambda_{k,\mathsf{eff}}^{\mathsf{Dir}}(\varepsilon) + \tilde{c}_0 \in \mathcal{Z}_{c_0,C_0,\varepsilon}.$$

As in the proof of Proposition 15.5 we obtain from Proposition 15.6 and the min-max principle

$$\left| \left(\lambda_k^{\mathsf{Dir}}(\varepsilon) - (\lambda_{k,\mathsf{eff}}^{\mathsf{Dir}}(\varepsilon) + \tilde{c}_0)\right)^{-1} - \left(\lambda_{k,\mathsf{eff}}^{\mathsf{Dir}}(\varepsilon) - (\lambda_{k,\mathsf{eff}}^{\mathsf{Dir}}(\varepsilon) + \tilde{c}_0)\right)^{-1} \right| = \mathcal{O}(\varepsilon).$$

We deduce

$$\left|\lambda_k^{\mathsf{Dir}}(\varepsilon) - \lambda_{k,\mathsf{eff}}^{\mathsf{Dir}}(\varepsilon)\right| = \mathcal{O}(\varepsilon)\left|\left(\lambda_k^{\mathsf{Dir}}(\varepsilon) - (\lambda_{k,\mathsf{eff}}^{\mathsf{Dir}}(\varepsilon) + \tilde{c}_0)\right)\right|\,,$$

and the conclusion follows. ☐

15.3.3 Dirichlet-Robin shell with large coupling constant

In this section, we keep considering the hypersurface Σ of the last paragraph (here $\varepsilon = 1$). Let us now consider the Dirichlet-Robin Laplacian in an annulus. In other words, with w_1 and G_1 as defined by (15.23) and (15.24), we consider on the weighted space $L^2(w_1\mathrm{d}s\mathrm{d}t)$ the quadratic form

$$\mathcal{Q}_\alpha^{\mathsf{DR}}(\psi) = \int_{\Sigma\times(0,1)} \left(\langle G_1(s,t)\nabla_s\psi, \nabla_s\psi\rangle_{T\Sigma} + |\partial_t\psi|^2\right) w_1(s,t)\mathrm{d}s\mathrm{d}t - \alpha\int_\Sigma |\psi(s,0)|^2\mathrm{d}s.$$

It is defined for $\psi \in \mathsf{Dom}(\mathcal{Q}_\alpha^{\mathsf{DR}})$ where

$$\mathsf{Dom}(\mathcal{Q}_\alpha^{\mathsf{DR}}) = \{\psi \in H^1(\Sigma\times(0,1)) : \psi(s,1) = 0\,, \quad \partial_t\psi(s,0) = -\alpha\psi(s,0)\}\,.$$

In these definitions α is real, and we are interested in the strong coupling limit $\alpha \to +\infty$.

This quadratic form is of the form (15.14) with $S = G_1^{\frac{1}{2}}\nabla_s$ and $T_s = -w_1^{-1}\partial_t w_1\partial_t$ acting on $H^2((0,1))$ and Dirichlet-Robin condition. The spectrum of T_s is well-understood in the limit $\alpha \to +\infty$. Actually, the family (T_s) depends analytically on the principal curvatures $(\kappa_j(s))_{1\leq j\leq d-1}$. We can deduce from the previous works [6, 7, 9] that, as $\alpha \to +\infty$,

$$\mu_1(s,\alpha) = -\alpha^2 - \alpha\kappa(s) + \mathcal{O}(1)\,, \quad \mu_2(s,\alpha) \geq c > 0\,,$$

and

$$\mu(\alpha) = \inf_{s\in\Sigma}\mu_1(s,\alpha) = -\alpha^2 - \alpha\kappa_{\max} + \mathcal{O}(1)\,,$$

with $\kappa = \sum_{j=1}^{d-1}\kappa_j$. Here, for simplicity, we assume that κ has a unique maximum at $s = 0$ that is not degenerate and not attained at infinity. Moreover, we assume that the eigenvalues of $D_s^2 + \frac{1}{2}\mathsf{Hess}_0(-\kappa)(s,s)$ are simple. We let

$$\mathcal{Z}_{C_0,c_0,\alpha} = \{z \in \mathbb{R} : |z - \mu(\alpha)| \leq c_0\alpha\,, \quad \mathrm{dist}(z, \mathsf{Sp}(\widehat{\mathscr{L}_\alpha^{\mathsf{DR}}})) \geq C_0\}\,.$$

Proposition 15.8. *There exist $C, \alpha_0 > 0$ such that, for all $z \in \mathcal{Z}_{C_0,c_0,\alpha}$*

$$\left\| \left(\mathscr{L}_\alpha^{\mathsf{DR}} - z\right)^{-1} - \left(\mathscr{L}_{\alpha,\mathsf{eff}}^{\mathsf{DR}} - z\right)^{-1} \right\| \leq C\alpha^{-1}\,.$$

Proof. Here we have $\gamma = \mathcal{O}(\alpha^2)$, $\nu = \mathcal{O}(\alpha^{-1})$ and $a = \mathcal{O}(\alpha^{-2})$. We use again Remark 15.1 and we apply Theorem 15.1 with $\mathscr{L} = \mathscr{L}_\alpha^{\mathsf{DR}} - \mu(\alpha)$ and z replaced by $z - \mu(\alpha)$. For $z \in \mathcal{Z}_{c_0,C_0,\alpha}$, we get

$$\eta_1 = \mathcal{O}(\alpha^{-1})\,, \quad \eta_2 = \mathcal{O}(\alpha^{-2})\,, \quad \eta_3 = \mathcal{O}(\alpha^{-2})\,, \quad \eta_4 = \mathcal{O}(\alpha^{-3})\,.$$

Moreover, for α large enough, we have, for all $z \in Z_{c_0,C_0,\alpha}$, $z \in \rho\left(\mathscr{L}_{\alpha,\mathsf{eff}}^{\mathsf{DR}}\right)$ and

$$\|(\mathscr{L}_{\alpha,\mathsf{eff}}^{\mathsf{DR}} - z)^{-1}\| \leq C\,.$$

Then Theorem 15.1 implies the wished estimate. □

We recover, under our simplifying assumptions, a result appearing in [6, 17, 9].

Proposition 15.9. *For all $j \geq 1$, we have, as $\alpha \to +\infty$,*

$$\lambda_{j,\mathsf{eff}}^{\mathsf{DR}}(\alpha) = -\alpha^2 + \nu_j(\alpha) + \mathcal{O}(1)\,,$$

and

$$\lambda_j^{\mathsf{DR}}(\alpha) = -\alpha^2 + \nu_j(\alpha) + \mathcal{O}(1)\,,$$

where $\nu_j(\alpha)$ is the j-th eigenvalue of $D_s^2 - \alpha\kappa(s)$.

Proof. Let us first discuss the asymptotic behavior of the eigenvalues of the effective operator. Let us recall that it is defined as explained in Section 15.1.2, and that it can be identified with the operator associated with the form $H^1(\Sigma) \ni \varphi \mapsto \mathcal{Q}_\alpha^{\mathsf{DR}}(\varphi u_{s,\alpha})$ where $u_{s,\alpha}$ is the positive L^2-normalized groundstate of the transverse operator $T(s)$. The asymptotic expansion of the effective eigenvalues again follows from perturbation theory and a commutator estimate (see [9, Section 3] where it is explained how we can estimate such a commutator).

Then, we proceed as in the previous section. Note that, by the harmonic approximation, for all $j \geq 1$,

$$\nu_j(\alpha) = -\alpha\kappa_{\max} + \alpha^{\frac{1}{2}}\tilde{\nu}_j + \mathcal{O}(\alpha^{\frac{1}{4}})\,,$$

where $(\tilde{\nu}_j)_{j\in\mathbb{N}^*}$ is the non-decreasing sequence of the eigenvalues of $D_s^2 + \frac{1}{2}\mathsf{Hess}_0(-\kappa)(s,s)$. In particular, the asymptotic gap between consecutive eigenvalues is of order $\alpha^{\frac{1}{2}}$. Then, there exist $c_0 > 0$, $C_0 > 0$ and $C > 0$ such that, for α large, $z = \lambda_{j,\mathsf{eff}}^{\mathsf{DR}}(\alpha) + C \in \mathcal{Z}_{c_0,C_0,\alpha}$. We use Proposition 15.8 and we get, as in the other examples,

$$|\lambda_{j,\mathsf{eff}}^{\mathsf{DR}}(\alpha) - \lambda_j^{\mathsf{DR}}(\alpha)| \leq C\alpha^{-1}\,.$$

□

15.4 The non-self-adjoint Robin Laplacian between hypersurfaces

In this section we prove Theorem 15.2. The proof is split in two main steps. We first transform the problem into an equivalent statement, where $\mathscr{P}_\varepsilon$ is replaced by a unitarily equivalent operator on Ω.

15.4.1 A change of variables

The operator $\mathscr{P}_\varepsilon$ is associated to the (coercive) quadratic form defined for $\phi \in H^1(\Omega_\varepsilon)$ by

$$Q_\varepsilon^1(\phi) = Q_{\varepsilon,\alpha}^1(\phi) = \int_{\Omega_\varepsilon} |\nabla\phi|^2 + \int_{\Sigma_{+,\varepsilon}} \alpha_{+,\varepsilon}|\phi|^2 - \int_{\Sigma_{-,\varepsilon}} \alpha_{-,\varepsilon}|\phi|^2\,. \tag{15.25}$$

As in Section 15.3.2, we use the diffeomorphism Θ_ε to see $\mathscr{P}_\varepsilon$ as an operator on $L^2(\Omega)$: for $\psi \in H^1(\Omega)$ we set

$$Q_\varepsilon^2(\psi) = Q_\varepsilon^1(\psi \circ \Theta_\varepsilon^{-1})\,.$$

We obtain

$$\begin{aligned}
Q^2_\varepsilon(\psi) &= \int_{\Omega_\varepsilon} |(\mathrm{Id}_{T_s\Sigma} + \varepsilon t d_s n)^{-1}\nabla_s \psi(\Theta_\varepsilon^{-1}(x))|^2\, dx + \frac{1}{\varepsilon^2}\int_{\Omega_\varepsilon} |\partial_t \psi(\Theta_\varepsilon^{-1}(x))|^2 \mathrm{d}x \\
&\quad + \int_{\Sigma_+} \alpha_{+,\varepsilon} |\psi \circ (\Theta_\varepsilon^+)^{-1}|^2 - \int_{\Sigma_-} \alpha_{-,\varepsilon}|\psi\circ(\Theta_\varepsilon^+)^{-1}|^2 \\
&= \int_\Omega \langle G_\varepsilon(s,t)\nabla_s\psi, \nabla_s\psi\rangle_{T\Sigma}\varepsilon\tilde{w}_\varepsilon \mathrm{d}\sigma\mathrm{d}t + \frac{1}{\varepsilon}\int_\Omega |\partial_t\psi|^2\tilde{w}_\varepsilon\mathrm{d}\sigma\mathrm{d}t \\
&\quad + \int_\Sigma \alpha\,(|\psi|^2\tilde{w}_\varepsilon)|_{t=1}\mathrm{d}\sigma - \int_\Sigma \alpha\,(|\psi|^2\tilde{w}_\varepsilon)|_{t=-1}\mathrm{d}\sigma,
\end{aligned}$$

where, as in (15.23), $\tilde{w}(s,t) = \prod_{j=1}^{d-1}(1-\varepsilon t\kappa_j(s))$. Notice that $L^2(\Omega, \mathrm{d}\sigma\mathrm{d}t)$ and $L^2(\Omega, \varepsilon\tilde{w}_\varepsilon\mathrm{d}\sigma\mathrm{d}t)$ (or their corresponding Sobolev spaces) are equal as sets, but Θ_ε induces only a unitary transformation from $L^2(\Omega,\varepsilon\tilde{w}_\varepsilon\mathrm{d}\sigma\mathrm{d}t)$ to $L^2(\Omega_\varepsilon, \mathrm{d}x)$.

15.4.2 A change of function

In the next step we make a change of function to turn our problem with Robin boundary conditions into an equivalent problem with Neumann boundary conditions. For this we consider the unitary transform

$$\tilde{U}_\varepsilon : \left\{ \begin{array}{ccc} L^2(\Omega, \varepsilon\tilde{w}_\varepsilon\mathrm{d}\sigma\mathrm{d}t) & \to & L^2(\Omega, e^{-2\varepsilon t\Re(\alpha)}\tilde{w}_\varepsilon\mathrm{d}\sigma\mathrm{d}t), \\ u & \mapsto & \sqrt{\varepsilon}e^{\alpha\varepsilon t}u. \end{array}\right.$$

We set

$$w_\varepsilon = e^{-2\varepsilon t\Re(\alpha)}\tilde{w}_\varepsilon\,.$$

Then on $H^1(\Omega, w_\varepsilon\mathrm{d}\sigma\mathrm{d}t)$ we consider the transformed quadratic form given by

$$\begin{aligned}
Q_\varepsilon(\phi) &= Q^2_\varepsilon(\tilde{U}^{-1}\phi) \\
&= \int_\Omega \langle G_\varepsilon(\nabla_s - \varepsilon t\nabla_s\alpha)\phi, (\nabla_s - \varepsilon t\nabla_s\alpha)\phi\rangle w_\varepsilon\mathrm{d}\sigma\mathrm{d}t + \frac{1}{\varepsilon^2}\int_\Omega |\partial_t\phi|^2 w_\varepsilon\mathrm{d}\sigma\mathrm{d}t \\
&\quad - \frac{1}{\varepsilon}\int_\Omega \left(\alpha\phi\partial_t\bar{\phi} + \bar{\alpha}\bar{\phi}\partial_t\phi\right)w_\varepsilon\mathrm{d}\sigma\mathrm{d}t + \int_\Omega |\alpha|^2|\phi|^2 w_\varepsilon\mathrm{d}\sigma\mathrm{d}t \\
&\quad + \frac{1}{\varepsilon}\int_\Sigma \alpha|\phi|w_\varepsilon\mathrm{d}\sigma - \frac{1}{\varepsilon}\int_\Sigma \alpha|\phi|^2 w_\varepsilon\mathrm{d}\sigma\,.
\end{aligned}$$

By integration by parts we have

$$\begin{aligned}
&-\frac{1}{\varepsilon}\int_\Omega \alpha\phi\partial_t\bar{\phi}w_\varepsilon\mathrm{d}\sigma\mathrm{d}t \\
&\qquad = -\frac{1}{\varepsilon}\int_\Sigma \alpha|\phi|w_\varepsilon\mathrm{d}\sigma + \frac{1}{\varepsilon}\int_\Sigma \alpha|\phi|^2 w_\varepsilon\mathrm{d}\sigma + \int_\Omega\left(-2\alpha\Re(\alpha) + \frac{\alpha\partial_t\tilde{w}_\varepsilon}{\varepsilon\tilde{w}_\varepsilon}\right)|\phi|^2 w_\varepsilon\mathrm{d}\sigma\mathrm{d}t\,.
\end{aligned}$$

Finally,

$$\begin{aligned}
Q_\varepsilon(\phi) &= \int_\Omega \langle G_\varepsilon(\nabla_s - \varepsilon t\nabla_s\alpha)\phi, (\nabla_s - \varepsilon t\nabla_s\alpha)\phi\rangle w_\varepsilon\mathrm{d}\sigma\mathrm{d}t + \frac{1}{\varepsilon^2}\int_\Omega |\partial_t\phi|^2 w_\varepsilon\mathrm{d}\sigma\mathrm{d}t \\
&\quad + \frac{2i}{\varepsilon}\int_\Omega \Im(\alpha)\partial_t\phi\bar{\phi}w_\varepsilon\mathrm{d}\sigma\mathrm{d}t + \int_\Omega V_\varepsilon|\phi|^2 w_\varepsilon\mathrm{d}\sigma\mathrm{d}t\,,
\end{aligned}$$

where

$$V_\varepsilon = |\alpha|^2 - 2\alpha\Re(\alpha) + \alpha\frac{\partial_t\tilde{w}_\varepsilon}{\varepsilon\tilde{w}_\varepsilon}\,.$$

On $H^1(\Omega, w_\varepsilon\mathrm{d}\sigma\mathrm{d}t)$ we can also consider the forms defined by

$$\widehat{Q}_\varepsilon(\phi) = \int_\Omega |\nabla_s\phi|^2\mathrm{d}\sigma\mathrm{d}t + \frac{1}{\varepsilon^2}\int_\Omega |\partial_t\phi|^2\mathrm{d}\sigma\mathrm{d}t + \int_\Omega V_{\mathsf{eff}}|\phi|^2\mathrm{d}\sigma\mathrm{d}t$$

and

$$Q_{\mathsf{eff}}(\phi) = \int_\Omega |\nabla_s\phi|^2\mathrm{d}\sigma\mathrm{d}t + \int_\Omega V_{\mathsf{eff}}|\phi|^2\mathrm{d}\sigma\mathrm{d}t.$$

We denote by $\mathscr{L}_\varepsilon$, $\widehat{\mathscr{L}_\varepsilon}$ and $\mathscr{L}_{\mathsf{eff}}$ the operators corresponding to the forms Q_ε, $\widehat{Q}_\varepsilon$ and Q_{eff}, respectively.

15.4.3 About the new operator $\mathscr{L}_\varepsilon$

If U_ε denotes the composition of the unitary transform associated with Θ_ε and $\tilde{U}_\varepsilon$, we write $\mathscr{L}_\varepsilon = U_\varepsilon \mathscr{P}_\varepsilon U_\varepsilon^{-1}$ and the estimate of Theorem 15.2 can be rewritten as

$$\|(\mathscr{L}_\varepsilon - z)^{-1} - (\mathscr{L}_{\mathsf{eff}} - z)^{-1}\Pi\|_{\mathcal{L}(L^2(\Omega))} \lesssim \varepsilon \,. \tag{15.26}$$

As $\mathscr{P}_\varepsilon$, the operator $\mathscr{L}_\varepsilon$ is m-accretive. We have the following accretivity estimate when ε goes to 0.

Lemma 15.6. *If $\varepsilon_0 > 0$ is small enough there exist $M_0 \geq 0$ and $c_0 > 0$ such that for $\varepsilon \in (0, \varepsilon_0)$, $M \geq M_0$ and $\phi \in H^1(\Omega)$ we have*

$$\Re\big(Q_\varepsilon(\phi)\big) + M\|\phi\|^2_{L^2(\Omega)} \geq c_0 \left(\|\nabla_s \phi\|^2_{L^2(\Omega)} + \frac{1}{\varepsilon^2}\|\partial_t \phi\|^2_{L^2(\Omega)} + \|\phi\|^2_{L^2(\Omega)} \right) .$$

Proof. There exists $C_1 \geq 0$ such that for $\varepsilon \in (0, \varepsilon_0)$ and $\phi \in H^1(\Omega)$ we have

$$\begin{aligned}\Re\big(Q_\varepsilon(\phi)\big) \geq (1 - C_1\varepsilon)\|(\nabla_s - \varepsilon t \nabla_s \alpha)\phi\|^2 + \frac{1 - C_1\varepsilon}{\varepsilon^2}\|\partial_t \phi\|^2 \\ - \frac{2\|\Im(\alpha)\|_\infty (1 + C_1\varepsilon)}{\varepsilon}\|\partial_t \phi\|\|\phi\| - C_1\|\phi\|^2.\end{aligned}$$

For some $C_2 \geq 0$ we also have

$$\|(\nabla_s - \varepsilon t \nabla \alpha)\phi\|^2 \geq (1 - \varepsilon)\|\nabla_s \phi\|^2 - C_2\|\phi\|^2 \,.$$

and

$$\begin{aligned}&\frac{1 - C_1\varepsilon}{\varepsilon^2}\|\partial_t \varphi\|^2 - \frac{2\|\Im(\alpha)\|_\infty (1 + C_1\varepsilon)}{\varepsilon}\|\partial_t \varphi\|\|\varphi\| \\ &\quad = (1 - C_1\varepsilon)\left(\frac{\|\partial_t \varphi\|^2}{\varepsilon^2} - \frac{\|\partial_t \varphi\|}{\varepsilon}\frac{2\|\Im(\alpha)\|_\infty (1 + C_1\varepsilon)\|\varphi\|}{1 - C_1\varepsilon} \right) \\ &\quad \geq (1 - C_1\varepsilon)\frac{\|\partial_t \varphi\|^2}{2\varepsilon^2} - C_2\|\varphi\|^2 \,.\end{aligned}$$

The conclusion follows if $\varepsilon_0 > 0$ was chosen small enough. □

A remarkable property of $\mathscr{L}_\varepsilon$ is the following complex symmetry (cf. [1]).

Lemma 15.7. *Let $\varepsilon > 0$ and $z \in \mathbb{C}$. If $z \in \mathbb{C}$ is an eigenvalue for $\mathscr{L}_\varepsilon$ then $\overline{z}$ is an eigenvalue for $\mathscr{L}_\varepsilon^*$. In particular the operator $\mathscr{L}_\varepsilon$ has no residual spectrum.*

Proof. Since $\mathscr{L}_\varepsilon$ is unitarily equivalent to $\mathscr{P}_\varepsilon = \mathscr{P}_{\varepsilon,\alpha}$, it is sufficient to prove the result for $\mathscr{P}_{\varepsilon,\alpha}$. Notice that $\mathsf{D}(Q^1_{\varepsilon,\alpha}) = \mathsf{D}(Q^1_{\varepsilon,\overline{\alpha}})$. Moreover for $\phi, \psi \in \mathsf{D}(Q^1_{\varepsilon,\alpha})$ we have $Q^1_{\varepsilon,\overline{\alpha}}(\phi,\psi) = \overline{Q^1_{\varepsilon,\alpha}(\psi,\phi)}$, so $\mathscr{P}^*_{\varepsilon,\alpha} = \mathscr{P}_{\varepsilon,\overline{\alpha}}$. Now let $\psi \in \mathsf{D}(\mathscr{P}_{\varepsilon,\alpha})$. For all $\phi \in \mathsf{D}(Q^1_{\varepsilon,\alpha})$ we have

$$Q^1_{\varepsilon,\overline{\alpha}}(\phi, \overline{\psi}) = \overline{Q^1_{\varepsilon,\alpha}(\overline{\phi}, \psi)} = \overline{\langle \overline{\phi}, \mathscr{P}_{\varepsilon,\alpha}\psi \rangle} = \langle \phi, \overline{\mathscr{P}_{\varepsilon,\alpha}\psi} \rangle \,.$$

This proves that $\overline{\psi} \in \mathsf{D}(\mathscr{P}_{\varepsilon,\overline{\alpha}})$ and $\mathscr{P}_{\varepsilon,\overline{\alpha}}\psi = \overline{\mathscr{P}_{\varepsilon,\alpha}\psi}$. Thus, if we denote by J the complex conjugation, we get that $\mathscr{P}_{\varepsilon,\alpha}$ is J-self-adjoint

$$\mathscr{P}_{\varepsilon,\overline{\alpha}} = J\mathscr{P}_{\varepsilon,\alpha}J.$$

The conclusion follows. □

15.4.4 Proof of Theorem 15.2

Theorem 15.2 will be a consequence of the following proposition.

Proposition 15.10. *There exist $\varepsilon_0, C > 0$ such that for all $\varepsilon \in (0, \varepsilon_0)$, $\varphi \in \mathsf{Dom}(\widehat{\mathscr{L}_\varepsilon^*})$ and $\psi \in \mathsf{Dom}(\mathscr{L}_\varepsilon)$,*

$$|Q_\varepsilon(\varphi, \psi) - \widehat{Q}_\varepsilon(\varphi, \psi)| \leq C\varepsilon\|\varphi\|_{\widehat{\mathscr{L}_\varepsilon^*}}\|\psi\|_{\mathscr{L}_\varepsilon} \,.$$

Proof. We set

$$\mathsf{D}_\varepsilon(\varphi,\psi) = Q_\varepsilon(\varphi,\psi) - \widehat{Q}_\varepsilon(\varphi,\psi)\,.$$

Using the Taylor formula, we get

$$|\mathsf{D}_\varepsilon(\varphi,\psi)| \lesssim \varepsilon\|\varphi\|_{H^1_s}\|\psi\|_{H^1_s} + \frac{1}{\varepsilon}\|\partial_t\varphi\|\|\partial_t\psi\| + \left|\frac{2}{\varepsilon}\int_\Omega \Im(\alpha)\partial_t\psi\bar{\varphi}w_\varepsilon \mathrm{d}\sigma\mathrm{d}t\right|,$$

where $\|\psi\|^2_{H^1_s} = \|\psi\|^2_{L^2(\Omega)} + \|\nabla_s\psi\|^2_{L^2(\Omega)}$. The most delicate term is the last one. We have

$$|Q_\varepsilon(t\Im(\alpha)\varphi,\psi) - \frac{1}{\varepsilon^2}\int \Im(\alpha)\partial_t(t\overline{\varphi})\partial_t\psi w_\varepsilon \mathrm{d}\sigma\mathrm{d}t| \lesssim \|\varphi\|_{H^1_s}\|\psi\|_{H^1_s} + \frac{1}{\varepsilon}\|\varphi\|\|\partial_t\psi\|,$$

so

$$|Q_\varepsilon(t\Im(\alpha)\varphi,\psi) - \frac{1}{\varepsilon^2}\int \Im(\alpha)\overline{\varphi}\partial_t\psi w_\varepsilon \mathrm{d}\sigma\mathrm{d}t| \lesssim \|\varphi\|_{H^1_s}\|\psi\|_{H^1_s} + \frac{1}{\varepsilon^2}\|\partial_t\varphi\|\|\partial_t\psi\| + \frac{1}{\varepsilon}\|\varphi\|\|\partial_t\psi\|\,.$$

Since $Q_\varepsilon(t\Im(\alpha)\varphi,\psi) = \langle t\Im(\alpha)\varphi, \mathscr{L}_\varepsilon\psi\rangle$, we obtain

$$\left|\frac{1}{\varepsilon}\int \Im(\alpha)\partial_t\psi\overline{\varphi}w_\varepsilon \mathrm{d}\sigma\mathrm{d}t\right| \lesssim \varepsilon\|\varphi\|_{H^1_s}\|\psi\|_{H^1_s} + \frac{1}{\varepsilon}\|\partial_t\varphi\|\|\partial_t\psi\| + \|\varphi\|\|\partial_t\psi\| + \varepsilon\|\mathscr{L}_\varepsilon\psi\|\|\varphi\|\,.$$

We conclude with Lemma 15.6. □

By Proposition 15.10, there exists $C \geq 0$ such that for $z \in K$, $\varphi \in \mathsf{Dom}((H^{\mathsf{eff}}_\varepsilon)^*)$ and $\psi \in \mathsf{Dom}(H_\varepsilon)$ we have

$$|Q^{\mathsf{eff}}_\varepsilon(\varphi,\psi) - z\langle\varphi,\psi\rangle - (Q_\varepsilon(\varphi,\psi) - z\langle\varphi,\psi\rangle)\,| \leq C\varepsilon\|\varphi\|_{(H^{\mathsf{eff}}_\varepsilon - z)^*}\|\psi\|_{H_\varepsilon - z}\,.$$

Finally, we apply Lemma 15.5 and Lemma 15.1, and Theorem 15.2 follows.

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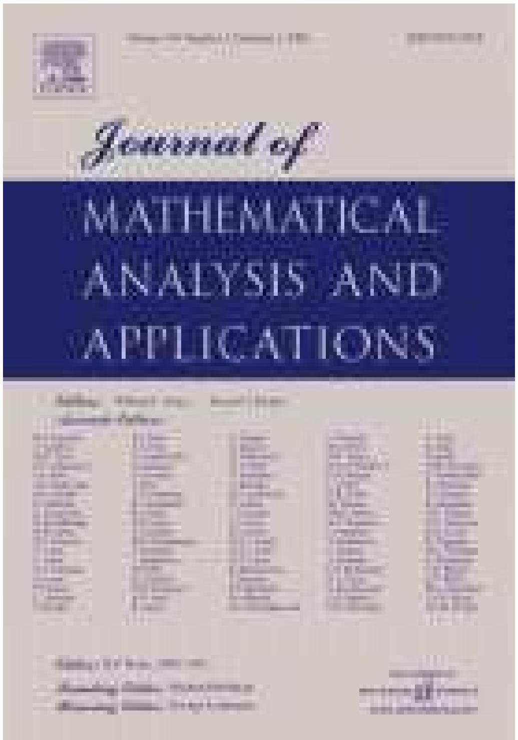
Chapter 16

Asymptotic spectral analysis in colliding leaky quantum layers



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Asymptotic spectral analysis in colliding leaky quantum layers

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Abstract. We consider the Schrödinger operator with a complex delta interaction supported by two parallel hypersurfaces in the Euclidean space of any dimension. We analyse spectral properties of the system in the limit when the distance between the hypersurfaces tends to zero. We establish the norm-resolvent convergence to a limiting operator and derive first-order corrections for the corresponding eigenvalues.

16.1 Introduction

Semiconductor heterostructures have had tremendous impact on science and technology as building blocks for a bottom-up approach to the fabrication of nanoscale devices. A key property of these material systems is the unique versatility in terms of geometrical dimensions and composition and their ability to exhibit quantum effects. Theoretical studies have lead to interesting mathematical problems which involve an interaction of differential geometry, spectral analysis and theory of partial differential equations. In this paper, we rely on the mathematical concept of *leaky quantum graphs* or *waveguides* introduced by Exner and Ichinose in 2001 [15] (see [14] for a survey), where the quantum Hamiltonian is modelled by the Schrödinger operator with a Dirac-measure potential supported on a hypersurface in $\mathbb{R}^d$.

The situations $d = 1, 2, 3$ are of particular interest in the context of mesoscopic physics of nanostructures, where they are sometimes referred to as *quantum dots*, *wires* or *layers*, respectively. We adopt the last terminology to emphasise the geometric complexity of the problem, but any value $d \geq 1$ is allowed in this paper. Using the Dirac-measure interaction instead of a regular potential to describe a quantum particle in a nanostructure is a simplification in the sense that the former vanishes outside the hypersurface. At the same time, it is a more realistic model than considering the particle confined to a tubular neighbourhood of the hypersurface by means of Dirichlet boundary conditions (see [12], [7], [31], [33] and [26] for this type of models in the case $d = 3$), because it takes into account *tunnelling*, property which is observed and measured in realistic heterostructures (see, *e.g.*, [6] and [9]).

The objective of this paper is to quantify the effect of tunnelling by considering coalescing heterostructures modelled by Dirac-measure potentials imposed on two parallel hypersurfaces separated by a distance ε and studying spectral properties in the limit as ε tends to zero. Spectral asymptotics of systems with leaky quantum waveguides have been analysed in various contexts and dimensions recently (see, *e.g.*, [3], [4], [5], [11], [17], [23], [32]). The geometric setting introduced in this paper is new and interesting both physically and mathematically. In fact, to establish the eigenvalue asymptotics as $\varepsilon \to 0$, we need to combine diverse methods of Riemannian geometry, spectral analysis and theory of partial differential equations.

Motivated by a growing interest in non-self-adjoint operators in recent years (*cf* the review article [29] and the book chapter [28] and references therein), in this paper we proceed in a great generality by allowing *complex* couplings on the colliding hypersurfaces. In quantum mechanics, non-self-adjoint operators are traditionally relevant as effective models of open systems and, more recently, as an unconventional representation of physical observables. Schrödinger operators with complex delta interactions are specifically used in Bose-Einstein condensates, where the imaginary part of the complex coupling models the injection and removal of particles (see [8] and [10]).

Let us now specify the mathematical model of this paper and present our main results. Let Ω be a bounded smooth open set in $\mathbb{R}^d$ with $d \geq 1$ and let us denote by $\Sigma_0 := \partial\Omega$ the boundary of Ω. For all sufficiently small positive ε, we consider parallel hypersurfaces

$$\Sigma_{\pm\varepsilon} := \{q \pm \varepsilon n(q) : q \in \Sigma_0\}, \tag{16.1}$$

where $n : \Sigma_0 \to \mathbb{R}^d$ denotes the outer unit normal to Ω. Finally, given two constants $\alpha_\pm \in \mathbb{C}$, we consider the operator in $L^2(\mathbb{R}^d)$ represented by the formal expression

$$H_\varepsilon := -\Delta + \alpha_+ \, \delta_{\Sigma_{+\varepsilon}} + \alpha_- \, \delta_{\Sigma_{-\varepsilon}}, \tag{16.2}$$

where δ_Σ denotes the Dirac delta function supported by a hypersurface $\Sigma \subset \mathbb{R}^d$. The purpose of this paper is to study spectral properties of H_ε in the limit when $\varepsilon \to 0$.

First of all, it is natural to expect that the limiting operator is given by

$$H_0 := -\Delta + (\alpha_+ + \alpha_-)\, \delta_{\Sigma_0} \,. \tag{16.3}$$

In this paper, we show that the convergence holds in the norm-resolvent sense.

Theorem 16.1. *For any $z \in \rho(H_0)$, there exists a positive constant ε_0 such that, for all $\varepsilon < \varepsilon_0$, we have $z \in \rho(H_\varepsilon)$ and*

$$\left\|(H_\varepsilon - z)^{-1} - (H_0 - z)^{-1}\right\|_{L^2(\mathbb{R}^d)\to L^2(\mathbb{R}^d)} = O(\varepsilon) \qquad as \qquad \varepsilon \to 0 \,. \tag{16.4}$$

As a consequence of Theorem 16.1, we obtain a convergence of the spectrum of H_ε to the spectrum of H_0 as $\varepsilon \to 0$. In particular, discrete eigenvalues change continuously with ε (*cf* [21, Sec. IV.3.5]). By a discrete eigenvalue λ_ε of H_ε we mean an isolated eigenvalue of finite algebraic multiplicity such that the range of $H_\varepsilon - \lambda_\varepsilon$ is closed. We remark that H_0 may or may not possess discrete eigenvalues, depending on the values of the coupling constants $\alpha_\pm$ and geometry of Σ_0; in particular, they always exist in the self-adjoint case if the constants are negative and sufficiently large. Since the interaction in (16.2) is compactly supported in $\mathbb{R}^d$, it is also possible to show that the essential spectrum of H_ε (*i.e.* the complement of the discrete eigenvalues in the spectrum) equals the essential spectrum of the self-adjoint Laplacian without the delta interactions, *i.e.*

$$\sigma_{\mathrm{ess}}(H_\varepsilon) = [0, +\infty) \,,$$

for all $\varepsilon \geq 0$, regardless of the geometry of Σ_0 and values of $\alpha_\pm$.

The main interest of Theorem 16.1 lies in the sharpness of the power of ε in (16.4). Indeed, as the next result of this paper, we derive the following asymptotics for simple eigenvalues.

Theorem 16.2. *Let λ_0 be a simple discrete eigenvalue of H_0 and let ψ_0 be the corresponding eigenfunction. There exist positive constants ε_0 and r such that, for all $\varepsilon < \varepsilon_0$, H_ε possesses precisely one discrete eigenvalue of algebraic multiplicity one in the open ball $B_r(\lambda_0)$ disk of radius r centred at λ_0. Moreover, the following asymptotics holds:*

$$\lambda_\varepsilon = \lambda_0 + \lambda_0' \, \varepsilon + O(\varepsilon^2) \qquad as \qquad \varepsilon \to 0 \tag{16.5}$$

with

$$\lambda_0' := \frac{\alpha_+ \displaystyle\int_{\Sigma_0} \partial_n^+ \psi_0^2 + \alpha_- \int_{\Sigma_0} \partial_n^- \psi_0^2 - \int_{\Sigma_0} \left[\alpha_+^2 + \alpha_-^2 + (\alpha_+ - \alpha_-)\,(d-1) K_1\right] \psi_0^2}{\displaystyle\int_{\mathbb{R}^d} \psi_0^2} \,, \tag{16.6}$$

where K_1 denotes the first mean curvature of Σ_0 and

$$\partial_n^\pm f(x) := \lim_{\epsilon \to 0^+} \frac{f(x \pm n\epsilon) - f(x)}{\epsilon} \,.$$

The functions appearing in the numerator of (16.6) should be understood in the sense of traces and their rigorous definition will be provided in the following section.

We also give an analogous theorem for degenerate semisimple eigenvalues, *i.e.* for the case when the algebraic and geometric multiplicity coincide, (*cf* [21, Sec. I.5.3]). This result is formulated as Theorem 16.4 below.

We remark that a presence of the first mean curvature in eigenvalue asymptotics has been recently observed in related problems, see [24], [25] and [34].

If $\alpha_+ = \alpha_-$, formula (16.6) simplifies to $\lambda_0' = 2\alpha_+^2$ (*cf* (16.15)), so the first correction term in the eigenvalue asymptotics is insensitive to the geometric setting if the coupling constants coincide.

We stress that the asymptotics (16.5) is not a consequence of analytic perturbation theory. As a matter of fact, taking a formal derivative of λ_ε with respect to ε in the spirit of the Hellmann-Feynman theorem would lead only to the first integral in the numerator of (16.6). Of course, this formal manipulation is not justified because of the singular dependence of H_ε on ε. It is interesting that a non-trivial rigorous approach is needed to reveal the geometric term in (16.6).

This paper is organised as follows. In Section 16.2 we present some necessary analytic and geometric prerequisites. The norm-resolvent convergence of Theorem 16.1 is established in Section 16.3. Our strategy is to derive first estimates for the norm of the resolvent as an operator between Sobolev spaces, which we believe are of interest on its own. In Section 16.4, we establish a uniform convergence of eigenfunctions by a refined application of the maximum principle. Section 16.5 is devoted to a proof of Theorem 16.2 as well as to its extension to degenerate eigenvalues. We conclude the paper by an appendix (Section 16.6), where Theorem 16.2 is re-established in the simplest case $d = 1$. Here the eigenvalue problem can be reduced to a transcendental equation, for which the implicit function theorem yields the the first correction term.

16.2 Preliminaries

Let us start by properly defining the operators H_ε and H_0 (the latter can be considered as H_ε for $\varepsilon = 0$ if we set $\Sigma_{\pm 0} := \Sigma_0$). The sum in (16.2) has a good meaning as a sum of bounded operators from the Sobolev space $H^1(\mathbb{R}^d)$ to its dual $H^{-1}(\mathbb{R}^d)$. It is more customary to consider H_ε as an unbounded operator in the Hilbert space $L^2(\mathbb{R}^d)$. To this purpose, we introduce the quadratic form

$$h_\varepsilon[\psi] := \int_{\mathbb{R}^d} |\nabla\psi|^2 + \alpha_+ \int_{\Sigma_{+\varepsilon}} |\psi|^2 + \alpha_- \int_{\Sigma_{-\varepsilon}} |\psi|^2 , \qquad \mathsf{D}(h_\varepsilon) := H^1(\mathbb{R}^d) , \tag{16.7}$$

which is formally associated with the expression on the right hand side of (16.2), and define H_ε as the unique m-sectorial operator associated with h_ε via the first representation theorem (*cf* [21, Thm. VI.2.1]).

The boundary terms in (16.7) should be understood in the sense of traces (*cf* [1]). More specifically, in analogy with (16.1), we introduce a mapping

$$\mathcal{L} : \Sigma_0 \times \mathbb{R} \to \mathbb{R}^d : \{(q,t) \mapsto q + t\, n(q)\} \tag{16.8}$$

and define sets $\Sigma_t := \mathcal{L}(\Sigma_0 \times \{t\})$. Because of the boundedness and smoothness of Ω, there exists a positive number a such that

$$\mathcal{L} : \Sigma_0 \times [-a,a] \to \mathcal{L}(\Sigma_0 \times [-a,a]) \text{ is a diffeomorphism.} \tag{16.9}$$

Consequently, Σ_t is a smooth hypersurface (parallel to Σ_0 at distance $|t|$) for all $|t| \le a$. (Neither Σ_0 nor Σ_t are necessarily connected.) By the trace embedding theorem (*cf* [1, Thm. 5.36]), the *trace operator*

$$\tau_t : H^1(\mathbb{R}^d) \to L^2(\Sigma_t) \tag{16.10}$$

is bounded for all $|t| \le a$. In fact, if $|t| \le a$, then for any $\delta > 0$ there exists a positive constant C_δ (depending in addition to δ also on the geometry of Σ_0) such that, for all $\psi \in H^1(\mathbb{R}^d)$,

$$\|\tau_t\psi\|^2_{L^2(\Sigma_t)} \le \delta\, \|\nabla\psi\|^2_{L^2(\mathbb{R}^d)} + C_\delta\, \|\psi\|^2_{L^2(\mathbb{R}^d)} . \tag{16.11}$$

This estimate can be proved in a standard way by using the diffeomorphism $\mathcal{L}$ and the one-dimensional bound

$$\sup_{(-l,l)} |\varphi|^2 \le 2\, \|\varphi\|_{L^2(-l,l)}\, \|\varphi'\|_{L^2(-l,l)} + (2l)^{-1}\, \|\varphi\|^2_{L^2(-l,l)} \tag{16.12}$$

valid for all $\varphi \in H^1((-l,l))$, where l is any positive number. It follows that the boundary terms in (16.7) (in which we ambiguously write ψ instead of $\tau_{\pm\varepsilon}\psi$) represent a relatively bounded perturbation of the gradient integral with the relative bound equal to zero (since δ can be taken arbitrarily small). Consequently, the form (16.7) is closed by classical perturbation results (*cf* [21, Thm. VI.1.33]), so that the first representation theorem applies.

Next we set

$$\begin{aligned} \Omega^0_\varepsilon &:= \{\mathcal{L}(q,t) : \, q \in \Sigma_0, \, -\varepsilon < t < +\varepsilon\} , \\ \Omega^\pm_\varepsilon &:= \{\mathcal{L}(q,t) : \, q \in \Sigma_0, \, \varepsilon < \pm t < a/2\} , \end{aligned} \tag{16.13}$$

where $0 \le \varepsilon < a/2$ (Ω^0_0 is an empty set). In words, Ω^0_ε (respectively, $\Omega^\pm_\varepsilon$) is the open set squeezed between the parallel hypersurfaces $\Sigma_{+\varepsilon}$ and $\Sigma_{-\varepsilon}$ (respectively, $\Sigma_{\pm\varepsilon}$ and $\Sigma_{\pm a/2}$). For positive ε, the trace operators

$$\begin{aligned} &\tau^-_{-\varepsilon} : H^2(\Omega^-_\varepsilon) \to H^1(\Sigma_{-\varepsilon}) , \quad \tau^+_{+\varepsilon} : H^2(\Omega^+_\varepsilon) \to H^1(\Sigma_{+\varepsilon}) , \\ &\tau^+_{-\varepsilon} : H^2(\Omega^0_\varepsilon) \to H^1(\Sigma_{-\varepsilon}) , \quad \tau^-_{+\varepsilon} : H^2(\Omega^0_\varepsilon) \to H^1(\Sigma_{+\varepsilon}) , \end{aligned} \tag{16.14}$$

are again bounded by the trace embedding theorem. The claim applies to the first line even if $\varepsilon = 0$. By using the first representation theorem and elliptic regularity theory, it is standard to show that H_ε acts as the Laplacian, subject to the interface conditions

$$\begin{cases} \tau^+_{\pm\varepsilon}\partial_n\psi - \tau^-_{\pm\varepsilon}\partial_n\psi = \alpha_\pm \tau_{\pm\varepsilon}\psi & \text{on} \quad \Sigma_{\pm\varepsilon} \quad \text{if} \quad \varepsilon > 0 , \\ \tau^+_{+0}\partial_n\psi - \tau^-_{-0}\partial_n\psi = (\alpha_+ + \alpha_-)\, \tau_0\psi & \text{on} \quad \Sigma_0 \quad \text{if} \quad \varepsilon = 0 . \end{cases} \tag{16.15}$$

More precisely, we have

$$\begin{aligned} H_\varepsilon\psi &= -\Delta\psi \qquad \text{a.e. in } \mathbb{R}^d , \\ \mathsf{D}(H_\varepsilon) &= \left\{\psi \in H^1(\mathbb{R}^d) \cap H^2\big(\mathbb{R}^d \setminus (\Sigma_{+\varepsilon} \cup \Sigma_{-\varepsilon})\big) : \psi \text{ satisfies (16.15)}\right\} . \end{aligned} \tag{16.16}$$

The meaning of the trace maps $\partial_n^{\pm}\psi \in L^2(\Sigma_0)$ used in formula (16.6) is precisely $\partial_n^{\pm}\psi := \pm\tau_{\pm 0}^{\pm}\partial_n\psi$.

Next, we overtake from [27] some facts about the geometry of parallel hypersurfaces. In view of (16.9), $\Omega_a := \mathcal{L}(\Sigma_0 \times (-a,a))$ can be identified with the Riemannian manifold $\Sigma_0 \times (-a,a)$ equipped with the metric G induced by (16.8); it has a block form

$$G(q,t) = g(q) \circ \big(I - t\,L(q)\big)^2 + \mathrm{d}t^2\,, \tag{16.17}$$

where g is the Riemannian metric of Σ_0, $L := -\mathrm{d}n$ is the Weingarten map of Σ_0 and I denotes the identity map on $T_q\Sigma_0$.

It follows from (16.17) that $|G| := \det(G) = |g|\,f^2$ with $|g| := \det(g)$ and

$$f(q,t) := \prod_{\mu=1}^{d-1}\big(1 - t\,\kappa_\mu(q)\big) = 1 + \sum_{\mu=1}^{d-1}(-t)^\mu \binom{d-1}{\mu} K_\mu(q)\,, \tag{16.18}$$

where $\kappa_1,\dots,\kappa_{d-1}$ are the *principal curvatures* and K_μ is the μ^{th} *mean curvature* of Σ_0 (*cf* [30]). Since the first mean curvature appears in Theorem 16.2, we remark that, locally,

$$K_1 = \frac{\kappa_1 + \cdots + \kappa_{d-1}}{d-1}\,.$$

The sign of K_1 depends on the orientation of Σ_0; in our case where Σ_0 is assumed to be oriented via the outer normal n to Ω, we have $K_1 \le 0$ if Ω is convex (*cf* [25]). It follows from (16.18) that the surface elements of Σ_0 and Σ_t are related by

$$\mathrm{d}\Sigma_t = f(q,t)\,\mathrm{d}\Sigma_0\,, \tag{16.19}$$

where $\mathrm{d}\Sigma_0 = |g(q)|^{1/2}\mathrm{d}q$.

From (16.9) and (16.18), we deduce

$$\forall |t| \le a\,, \quad t\,\max\{\|\kappa_1\|_\infty,\dots,\|\kappa_{d-1}\|_\infty\} < 1\,, \tag{16.20}$$

so that $\inf_{q\in\Sigma_0} f(q,t) > 0$ for every t such that $|t| \le a$. In particular, there exists a positive constant C (depending on a and the supremum norms of the principal curvatures) such that, for all $(q,t) \in \Sigma_0 \times [-a,a]$,

$$C^{-1} \le f(q,t) \le C \tag{16.21}$$

and

$$C^{-1}\,g(q) + \mathrm{d}t^2 \le G(q,t) \le C\,g(q) + \mathrm{d}t^2\,. \tag{16.22}$$

(Hereafter we adopt the convention that C denotes a generic constant whose value can change from line to line.)

Given a coordinate system $(q,t) \in \Sigma_0 \times (-a,a)$, we denote by G_{ij} and G^{ij} the corresponding coefficients of G and G^{-1}. We also adopt the Einstein summation convention, the range of Latin and Greek indices being $1,\dots,d$ and $1\dots d-1$, respectively, and abbreviate $\partial_i := \partial/\partial q^i$ with $q^d := t$ (we shall also write $\partial_t := \partial_d$). It will be convenient to choose for $q = (q^1,\dots,q^{d-1})$ the Riemannian normal coordinates in Σ_0, which exist in a neighbourhood of any point of Σ_0. In these coordinates, since Ω is smooth and bounded, there exists a positive number r_0 such that, for any $p \in \Sigma_0$, the useful estimates

$$C^{-1}\,(\delta_{\mu\nu}) \le (g_{\mu\nu}) \le C\,(\delta_{\mu\nu})\,, \qquad |\partial_\rho\, g_{\mu\nu}| \le C\,, \tag{16.23}$$

hold in the geodesic ball of radius r_0 centred at p.

Finally, we remark that the mapping (16.8) induces a natural unitary transform between Hilbert spaces

$$\mathcal{U} : L^2(\Omega_a) \to L^2\left(\Sigma_0 \times (-a,a), |G(q,t)|^{1/2}\,\mathrm{d}q \wedge \mathrm{d}t\right) : \{\psi \mapsto \psi \circ \mathcal{L}\}\,. \tag{16.24}$$

In particular, it will enable us to relate $L^2(\Sigma_t)$ and $L^2(\Sigma_0)$. Since H_ε acts as the Laplacian in $\mathbb{R}^d \setminus (\Sigma_{+\varepsilon} \cup \Sigma_{-\varepsilon})$, its action in the curvilinear "coordinates" (q,t) induced by $\mathcal{L}$ is given by Laplace-Beltrami operator

$$-\Delta_G := -|G|^{-1/2}\partial_i |G|^{1/2} G^{ij}\,\partial_j \tag{16.25}$$

in $\Sigma_0 \times [(-a,-\varepsilon) \cup (-\varepsilon,\varepsilon) \cup (\varepsilon,a)]$. Given $\psi \in L^2(\mathbb{R}^d)$, we shall occasionally write $\mathcal{U}\psi$, meaning that $\mathcal{U}$ acts on the restriction of ψ to $L^2(\Omega_a)$. We point out the following topological equivalence of Sobolev spaces.

Lemma 16.1. *There exists a positive constant C such that, for every $a \le t_1 < t_2 \le a$,*

$$C^{-1} \|\mathcal{U}\psi\|_{H^2(\Sigma_0\times(t_1,t_2))} \le \|\psi\|_{H^2(\mathcal{L}(\Sigma_0\times(t_1,t_2)))} \le C \|\mathcal{U}\psi\|_{H^2(\Sigma_0\times(t_1,t_2))}$$

for every $\psi \in H^2(\mathcal{L}(\Sigma_0 \times (t_1,t_2)))$.

Proof. The proof is a straightforward application of (16.8), namely (16.17) with estimates (16.23). We leave the details to the reader. □

Remark 16.1. Our assumptions about the regularity of Ω are far from being optimal. To introduce H_ε as an m-sectorial operator satisfying the natural characterisation (16.16), we essentially use the boundedness of the trace embeddings (16.14) together with standard elliptic regularity theory. It obviously works if Ω is bounded and smooth (*i.e.* infinitely smooth) as we assume in this paper. However, it is clear that a C^2-smoothness is sufficient and certain unbounded geometries can be included as well. In fact, a fundamental assumption is the validity of the diffeomorphism property (16.9). In the proofs, we essentially use that the eigenfunctions of H_ε are classical solutions of the associated partial differential equation. From another perspective, it should be also possible to modify the techniques of the present paper to handle the more general situation of $\alpha_\pm$ being C^1-smooth functions instead of constants.

16.3 The norm-resolvent convergence

The objective of this section is to prove Theorem 16.1. For all $\varepsilon \ge 0$ small enough and $z \in \rho(H_\varepsilon)$, we set

$$R_\varepsilon(z) := (H_\varepsilon - z)^{-1}\,.$$

Given $\Psi \in L^2(\mathbb{R}^d)$, the function $\psi_\varepsilon := R_\varepsilon(z)\Psi$ is the unique solution of the resolvent equation $(H_\varepsilon - z)\psi_\varepsilon = \Psi$. The weak formulation of the problem reads

$$\forall \varphi \in H^1(\mathbb{R}^d)\,, \qquad h_\varepsilon(\varphi,\psi_\varepsilon) - z\,(\varphi,\psi_\varepsilon)_{L^2(\mathbb{R}^d)} = (\varphi,\Psi)_{L^2(\mathbb{R}^d)}\,, \tag{16.26}$$

where $h_\varepsilon(\cdot,\cdot)$ is the sesquilinear form associated with (16.7).

First of all, we show that the resolvent $R_\varepsilon(z)$ is uniformly bounded as $\varepsilon \to 0$.

Lemma 16.2. *There exist constants $z_0 \in \mathbb{R}$ and $C > 0$ such that, for all $0 \le \varepsilon < a$ and every $z \in \mathbb{C}$ such that $\Re z < z_0$, $z \in \rho(H_\varepsilon)$ and*

$$\|R_\varepsilon(z)\|_{L^2(\mathbb{R}^d)\to H^1(\mathbb{R}^d)} \le C\,. \tag{16.27}$$

Proof. Since H_ε is m-sectorial, we know that the claim holds with an *a priori* ε-dependent constant z_0. The content of the lemma is that z_0 can be made actually independent of ε. Choosing the test function $\varphi := \psi_\varepsilon$ in (16.26), taking the real part of the obtained identity and applying (16.11) together with the Schwarz inequality, we get

$$[1 - \delta\,(|\Re\alpha_+| + |\Re\alpha_-|)]\,\|\nabla\psi_\varepsilon\|^2_{L^2(\mathbb{R}^d)} - [C_\delta\,(|\Re\alpha_+| + |\Re\alpha_-|) + \Re z]\,\|\psi_\varepsilon\|^2_{L^2(\mathbb{R}^d)} \le \|\psi_\varepsilon\|_{L^2(\mathbb{R}^d)}\,\|\Psi\|_{L^2(\mathbb{R}^d)}\,.$$

We choose δ so small that $1-\delta\,(|\Re\alpha_+|+|\Re\alpha_-|) \ge 1/2$. It follows that every $z \in \mathbb{C}$ such that $\Re z < -C_\delta\,(|\Re\alpha_+|+|\Re\alpha_-|)$ lies outside the closure of the numerical range of H_ε, that is, inside the resolvent set $\rho(H_\varepsilon)$ because H_ε is m-sectorial. Choosing

$$z_0 := -\frac{1}{2} - C_\delta\,(|\Re\alpha_+| + |\Re\alpha_-|)\,, \tag{16.28}$$

we arrive at (16.27) with $C := \sqrt{8}$. □

Remark 16.2. It is also possible to look for solutions of (16.26) for $\Psi \in H^{-1}(\mathbb{R}^d)$ in which case the right hand side must be understood as the duality pairing between $H^1(\mathbb{R}^d)$ and $H^{-1}(\mathbb{R}^d)$. Proceeding as in the previous proof, with a slight modification that the Schwarz inequality is replaced by the estimate

$$\left|{}_{H^1(\mathbb{R}^d)}(\psi_\varepsilon,\Psi)_{H^{-1}(\mathbb{R}^d)}\right| \le \|\psi_\varepsilon\|_{H^1(\mathbb{R}^d)}\,\|\Psi\|_{H^{-1}(\mathbb{R}^d)}\,,$$

we obtain

$$\|R_\varepsilon(z)\|_{H^{-1}(\mathbb{R}^d)\to H^1(\mathbb{R}^d)} \le C$$

with $C := 2$.

We shall need a resolvent estimate of the type (16.27) in a better topology. In the case of the free Hamiltonian (*i.e.* $\alpha_\pm = 0$), we know that the resolvent is bounded in the topology of bounded operators on $L^2(\mathbb{R}^d)$ to $H^2(\mathbb{R}^d)$. It does not hold if α_+ or α_- is non-zero, because then the functions from the domain of H_ε are not in $H^2(\mathbb{R}^d)$, *cf* (16.16). However, the functions belong to $H^2(\mathbb{R}^d \setminus (\Sigma_{+\varepsilon} \cup \Sigma_{-\varepsilon}))$ and the following uniform estimate holds.

Lemma 16.3. *There exists a positive constant C such that, for every $z \in \mathbb{C}$ satisfying $\Re z < z_0$ with z_0 given by* (16.28) *and for all $0 \leq \varepsilon < a/4$, we have*

$$\|R_\varepsilon(z)\|_{L^2(\mathbb{R}^d)\to H^2(\mathbb{R}^d\setminus(\Sigma_{+\varepsilon}\cup\Sigma_{-\varepsilon}))} \leq C\,. \tag{16.29}$$

Proof. The message of the lemma is that the constant C in (16.29) can be made independent of ε, which is not *a priori* clear. Setting $\psi_\varepsilon := R_\varepsilon(z)\Psi$ for every $\Psi \in L^2(\mathbb{R}^d)$ as above (recall that ψ_ε satisfies (16.26)), estimate (16.29) is equivalent to the simultaneous validity of the bounds

$$\|\psi_\varepsilon\|_{H^2(\Omega_\varepsilon^0)} \leq C\,\|\Psi\|_{L^2(\mathbb{R}^d)}\,, \tag{16.30}$$

$$\|\psi_\varepsilon\|_{H^2(\Omega_\varepsilon^\pm)} \leq C\,\|\Psi\|_{L^2(\mathbb{R}^d)}\,, \tag{16.31}$$

$$\|\psi_\varepsilon\|_{H^2(\mathbb{R}^d\setminus\overline{\Omega_{a/4}^0})} \leq C\,\|\Psi\|_{L^2(\mathbb{R}^d)}\,, \tag{16.32}$$

with a constant C independent of Ψ and ε. Here the sets $\Omega_\varepsilon^\pm$ and Ω_ε^0 are defined in (16.13). Note that $\psi_\varepsilon \in H^2(\mathbb{R}^d \setminus (\Sigma_{+\varepsilon} \cup \Sigma_{-\varepsilon}))$ is known due to (16.16); our aim is to establish the uniform estimates (16.30)–(16.32).

Estimate (16.32) follows at once by the interior regularity of weak solutions of the elliptic problem $(H_\varepsilon - z)\psi_\varepsilon = \Psi$ in $\Omega' := \mathbb{R}^d \setminus \overline{\Omega_{a/4}^0}$; see, *e.g.*, [13, Thm. 6.3.1] together with Lemma 16.2, recall that H_ε acts as the Laplacian in Ω' due to (16.16) and notice that Ω' is independent of ε. The validity of (16.30) and (16.31) is less obvious because of the ε-dependent interface conditions (16.15) and, consequently, a refined boundary regularity is needed. Let us sketch the proof of (16.30) with $\varepsilon > 0$. The proof of (16.31) with $\varepsilon \geq 0$ is analogous. Our approach is based on elliptic regularity; see, *e.g.*, [13, Sec. 6.3] to where we refer for more details.

Recalling (16.24), we set $v_\varepsilon := \mathcal{U}\psi_\varepsilon$ and $V := \mathcal{U}\Psi$. Let $\eta : \mathbb{R} \to [0,1]$ be a smooth cut-off function, which is equal to 1 on $(-a/2, a/2)$ and to 0 outside $(-3a/4, 3a/4)$ (we keep to denote by the same symbol η the function $1 \otimes \eta$ on $\Sigma_0 \times (-a,a)$). In (16.26), let us choose the test function φ in the following way

$$(\mathcal{U}\varphi)(q,t) := \eta(t)^2\, u(q,t)\,,$$

where $u \in H^1(\Sigma_0 \times (-a,a))$. Using (16.8), the identity (16.26) is transferred to

$$\begin{aligned}\big(\partial_i(\eta^2 u), G^{ij}\partial_j v_\varepsilon\big)_{\mathcal{H}} + \alpha_+ \int_{\Sigma_0} (\bar{u} v_\varepsilon f)(q,\varepsilon)\,\mathrm{d}\Sigma_0 + \alpha_- \int_{\Sigma_0} (\bar{u} v_\varepsilon f)(q,-\varepsilon)\,\mathrm{d}\Sigma_0 \\ - z\,\big(\eta^2 u, v_\varepsilon\big)_{\mathcal{H}} = \big(\eta^2 u, V\big)_{\mathcal{H}}\,,\end{aligned} \tag{16.33}$$

where $\mathcal{H}$ denotes the target Hilbert space in (16.24).

In (16.33), we choose

$$u(q,t) := -\partial_\rho^{-h}\partial_\rho^h v_\varepsilon(q,t)\,, \tag{16.34}$$

where $\rho \in \{1, \dots, d-1\}$ and $\partial_\rho^h v_\varepsilon(q,t)$ is the ρ^{th} difference quotient of size $h > 0$ (*cf* [13, Sec. 5.8.2])

$$\partial_\rho^h v_\varepsilon(q,t) := \frac{v_\varepsilon(q^1, \dots, q^\alpha + h, \dots q^{d-1}, t) - v_\varepsilon(q,t)}{h}\,.$$

Using the "integration-by-parts" rule for the difference quotients (*cf* [13, proof of Thm. 5.8.3]) and sending h to zero, we get

$$\begin{aligned}\big(\partial_i\partial_\rho v_\varepsilon, \eta^2 G^{ij}\partial_j\partial_\rho v_\varepsilon\big)_{\mathcal{H}} + \alpha_+ \int_{\Sigma_0} |\partial_\rho v_\varepsilon|^2(q,\varepsilon)\,\mathrm{d}\Sigma_0 + \alpha_- \int_{\Sigma_0} |\partial_\rho v_\varepsilon|^2(q,-\varepsilon)\,\mathrm{d}\Sigma_0 \\ + b[v_\varepsilon] + z\,\big(\eta^2\partial_\rho^2 v_\varepsilon, v_\varepsilon\big)_{\mathcal{H}} = -\big(\eta^2\partial_\rho^2 v_\varepsilon, V\big)_{\mathcal{H}}\,.\end{aligned} \tag{16.35}$$

Here $b[v_\varepsilon]$ is a quadratic form gathering subdominant terms that can be treated as a perturbation of the first line in (16.35) or integrals involving only first-order derivatives of v_ε. Recall that, by Lemma 16.2 and (16.22), we already know that

$$\|v_\varepsilon\|_{H^1(\Sigma_0\times(-a,a))} \leq C\,\|\Psi\|_{L^2(\mathbb{R}^d)}\,. \tag{16.36}$$

Writing

$$\left|\left(\eta^2\partial_\rho^2 v_\varepsilon, v_\varepsilon\right)_{\mathcal{H}}\right| \le \delta\, \|\eta\, \partial_\rho^2 v_\varepsilon\|_{\mathcal{H}}^2 + \delta^{-1}\, \|v_\varepsilon\|_{\mathcal{H}}^2$$
$$\left|\left(\eta^2\partial_\rho^2 v_\varepsilon, V\right)_{\mathcal{H}}\right| \le \delta\, \|\eta\, \partial_\rho^2 v_\varepsilon\|_{\mathcal{H}}^2 + \delta^{-1}\, \|V\|_{\mathcal{H}}^2\,,$$

the first terms on the right hand side with sufficiently small positive δ can be treated as a perturbation of the first dominant term of (16.35), while we have $\|V\|_{\mathcal{H}} = \|\Psi\|_{L^2(\Omega_a)} \le \|\Psi\|_{L^2(\mathbb{R}^d)}$ and (16.36). In fact, the boundary terms in (16.35) are also perturbations because of the following estimate based on (16.12):

$$\left|\int_{\Sigma_0} |\partial_\rho v_\varepsilon|^2(q,\pm\varepsilon)\, \mathrm{d}\Sigma_0\right| \le \delta\, \|\partial_t\partial_\rho v_\varepsilon\|_{L^2(\Sigma_0\times(-a/2,a/2))}^2 + (\delta^{-1}+a^{-1})\, \|\partial_\rho v_\varepsilon\|_{L^2(\Sigma_0\times(-a/2,a/2))}^2\,.$$

Summing up, from (16.35) with help of (16.36) together with (16.22) and (16.23), we conclude with key estimates

$$\|\partial_i\partial_\rho v_\varepsilon\|_{L^2(\Sigma_0\times(-a/2,a/2))} \le C\, \|\Psi\|_{L^2(\mathbb{R}^d)} \tag{16.37}$$

for every $i\in\{1,\dots,d\}$ and $\rho\in\{1,\dots,d-1\}$.

To get an analogous estimate for $\partial_t^2 v_\varepsilon$, we employ the fact that, by (16.16) and (16.8), v_ε satisfies the differential equation (recall (16.25))

$$-\,|G|^{-1/2}\partial_i(|G|^{1/2}G^{ij}\partial_j v_\varepsilon) - z\, v_\varepsilon = V \qquad \text{a.e. in } \Sigma_0\times(-\varepsilon,\varepsilon). \tag{16.38}$$

Using the block-diagonal structure of G, see (16.17), we can cast (16.38) into the form

$$-\,\partial_t^2 v_\varepsilon = V + z\, v_\varepsilon + |G|^{-1/2}\partial_\mu(|G|^{1/2}G^{\mu\nu}\partial_\nu v_\varepsilon) + |G|^{-1/2}(\partial_t|G|^{1/2})\partial_t v_\varepsilon\,, \tag{16.39}$$

where the right hand side contains no second-order derivative of v_ε with respect to t. Using (16.37) and (16.36), we can thus conclude with the missing inequality

$$\|\partial_t^2 v_\varepsilon\|_{L^2(\Sigma_0\times(-\varepsilon,\varepsilon))} \le C\, \|\Psi\|_{L^2(\mathbb{R}^d)}\,. \tag{16.40}$$

From (16.37) and (16.40) together with the first-order derivative inequality (16.36), we have thus obtained the estimate $\|v_\varepsilon\|_{H^2(\Sigma_0\times(-\varepsilon,\varepsilon))} \le C\, \|\Psi\|_{L^2(\mathbb{R}^d)}$. By Lemma 16.1, we then get an analogous estimate for $\psi_\varepsilon = \mathcal{U}^{-1}v_\varepsilon$ in the Euclidean set $\Omega_\varepsilon^0 = \mathcal{L}(\Sigma_0\times(-\varepsilon,\varepsilon))$. This concludes the sketch of the proof of (16.30) with $\varepsilon > 0$. $\square$

Now we are in a position to prove Theorem 16.1.

Proof of Theorem 16.1. Let $z\in\mathbb{C}$ be such that $\Re z < z_0$, where z_0 is given by (16.28), and $0<\varepsilon<a/4$. By Lemma 16.2, $z\in\rho(H_\varepsilon)$ for all $\varepsilon\ge 0$. Given any $\Phi,\Psi\in L^2(\mathbb{R}^d)$, we set $\psi_\varepsilon := R_\varepsilon(z)\Psi$ as before and $\phi_0 := R_0(z)^*\Phi$. We have

$$\begin{aligned}(\Phi,[R_\varepsilon(z)-R_0(z)]\Psi)_{L^2(\mathbb{R}^d)} &= ((H_0^*-\bar z)\phi_0,\psi_\varepsilon)_{L^2(\mathbb{R}^d)} - (\phi_0,(H_\varepsilon-z)\psi_\varepsilon)_{L^2(\mathbb{R}^d)}\\ &= h_0(\phi_0,\psi_\varepsilon) - h_\varepsilon(\phi_0,\psi_\varepsilon)\\ &= \alpha_+\left[(\phi_0,\psi_\varepsilon)_{L^2(\Sigma_0)} - (\phi_0,\psi_\varepsilon)_{L^2(\Sigma_{+\varepsilon})}\right]\\ &\quad + \alpha_-\left[(\phi_0,\psi_\varepsilon)_{L^2(\Sigma_0)} - (\phi_0,\psi_\varepsilon)_{L^2(\Sigma_{-\varepsilon})}\right],\end{aligned} \tag{16.41}$$

where the second equality employs the fact that the form domains of H_ε and H_0 coincide. The boundary terms after the last equality should be interpreted in the sense of traces (16.10).

The unitary transform (16.24) enables us to identify $L^2(\Sigma_{\pm\varepsilon})$ with $L^2(\Sigma_0)$. Writing $u_0 := \mathcal{U}\phi_0$ and $v_\varepsilon := \mathcal{U}\psi_\varepsilon$ and recalling (16.19), we have

$$\begin{aligned}&(\phi_0,\psi_\varepsilon)_{L^2(\Sigma_0)} - (\phi_0,\psi_\varepsilon)_{L^2(\Sigma_{+\varepsilon})}\\ &\quad= \int_{\Sigma_0}(\bar u_0 v_\varepsilon)(q,0)\,\mathrm{d}\Sigma_0 - \int_{\Sigma_0}(\bar u_0 v_\varepsilon)(q,\varepsilon)\, f(q,\varepsilon)\,\mathrm{d}\Sigma_0\\ &\quad= \underbrace{-\int_{\Sigma_0\times(0,\varepsilon)}\partial_t(\bar u_0 v_\varepsilon)(q,t)\,\mathrm{d}\Sigma_0\wedge\mathrm{d}t}_{I_1} + \underbrace{\int_{\Sigma_0}(\bar u_0 v_\varepsilon)(q,\varepsilon)\,[1-f(q,\varepsilon)]\,\mathrm{d}\Sigma_0}_{I_2}\,.\end{aligned}$$

Here the last integral can be estimated as follows

$$|I_2| \leq \|\phi_0\|_{L^2(\Sigma_{+\varepsilon})} \|\psi_\varepsilon\|_{L^2(\Sigma_{+\varepsilon})} \sup_{q\in\Sigma_0} \frac{|1-f(q,\varepsilon)|}{f(q,\varepsilon)}$$
$$\leq C\,\|\phi_0\|_{H^1(\mathbb{R}^d)} \|\psi_\varepsilon\|_{H^1(\mathbb{R}^d)} \sup_{q\in\Sigma_0} \frac{|1-f(q,\varepsilon)|}{f(q,\varepsilon)},$$

where the second inequality is due to (16.11). Taking into account the explicit formula for f in (16.18) and (16.21), we see that there is a constant C (depending on the geometric number a and the supremum norms of the curvature functions K_μ) such that

$$\sup_{q\in\Sigma_0} \frac{|1-f(q,\varepsilon)|}{f(q,\varepsilon)} \leq C\,\varepsilon\,. \tag{16.42}$$

By Lemma 16.2, we have

$$\|\psi_\varepsilon\|_{H^1(\mathbb{R}^d)} \leq C\,\|\Psi\|_{L^2(\mathbb{R}^d)} \qquad \text{and} \qquad \|\phi_0\|_{H^1(\mathbb{R}^d)} \leq C\,\|\Phi\|_{L^2(\mathbb{R}^d)}\,. \tag{16.43}$$

Since ϕ_0 is defined via the adjoint of the resolvent of H_0, it might be useful to mention for the latter inequality that H_0 satisfies the $\mathcal{T}$-self-adjointness relation $H_0^* = \mathcal{T}H_0\mathcal{T}$, where $\mathcal{T}$ is the complex-conjugation operator. Summing up,

$$|I_2| \leq C\,\varepsilon\,\|\Phi\|_{L^2(\mathbb{R}^d)}\,\|\Psi\|_{L^2(\mathbb{R}^d)}\,. \tag{16.44}$$

We now turn to estimating I_1. First of all, we use the Schwarz inequality to get

$$|I_1| \leq \|u_0\|_{L^2(\Sigma_0\times(0,\varepsilon))}\|\partial_t v_\varepsilon\|_{L^2(\Sigma_0\times(0,\varepsilon))} + \|\partial_t u_0\|_{L^2(\Sigma_0\times(0,\varepsilon))}\|v_\varepsilon\|_{L^2(\Sigma_0\times(0,\varepsilon))}\,.$$

Here the first term on the right hand side can be estimated as follows

$$\|u_0\|^2_{L^2(\Sigma_0\times(0,\varepsilon))} \leq \varepsilon \sup_{t\in(0,\varepsilon)} \int_{\Sigma_0} |u_0(q,t)|^2\,\mathrm{d}\Sigma_0 \leq C\,\varepsilon \sup_{t\in(0,\varepsilon)} \int_{\Sigma_t} |\phi_0|^2\,,$$

where $C := 1/\inf_{\Sigma_0\times(0,a)} f$. Using in addition (16.11) and (16.43), we eventually obtain

$$\|u_0\|_{L^2(\Sigma_0\times(0,\varepsilon))} \leq C\,\sqrt{\varepsilon}\,\|\Phi\|_{L^2(\mathbb{R}^d)}\,.$$

In the same manner, we get

$$\|v_\varepsilon\|_{L^2(\Sigma_0\times(0,\varepsilon))} \leq C\,\sqrt{\varepsilon}\,\|\Psi\|_{L^2(\mathbb{R}^d)}\,.$$

The terms $\|\partial_t v_\varepsilon\|_{L^2(\Sigma_0\times(0,\varepsilon))}$ and $\|\partial_t u_0\|_{L^2(\Sigma_0\times(0,\varepsilon))}$ require a bit more careful analysis. As above, we write

$$\|\partial_t u_0\|^2_{L^2(\Sigma_0\times(0,\varepsilon))} \leq \varepsilon \sup_{t\in(0,\varepsilon)} \int_{\Sigma_0} |\partial_t u_0(q,t)|^2\,\mathrm{d}\Sigma_0 \leq C\,\varepsilon \sup_{t\in(0,\varepsilon)} \int_{\Sigma_t} |\partial_n\phi_0|^2\,,$$

where we have also used $\partial_t u_0 = \partial_n\phi_0 \circ \mathcal{L}$. Now, however, we cannot use (16.11) because ϕ_0 is not in $H^2(\mathbb{R}^d)$. Nevertheless, it belongs to $H^2(\Omega_0^+)$, where the set Ω_0^+ is defined in (16.13). Hence,

$$\sup_{t\in(0,\varepsilon)} \int_{\Sigma_t} |\partial_n\phi_0|^2 \leq \sup_{t\in(0,a/2)} \int_{\Sigma_t} |\partial_n\phi_0|^2 \leq C\,\|\phi_0\|^2_{H^2(\Omega_0^+)}\,,$$

where the last inequality is a trace embedding based on (16.12). Applying Lemma 16.3, we eventually get the desired bound

$$\|\partial_t u_0\|_{L^2(\Sigma_0\times(0,\varepsilon))} \leq C\,\sqrt{\varepsilon}\,\|\Phi\|_{L^2(\mathbb{R}^d)}\,.$$

It remains to estimate $\|\partial_t v_\varepsilon\|_{L^2(\Sigma_0\times(0,\varepsilon))}$. Still, as above, we could also write

$$\|\partial_t v_\varepsilon\|^2_{L^2(\Sigma_0\times(0,\varepsilon))} \leq \varepsilon \sup_{t\in(0,\varepsilon)} \int_{\Sigma_0} |\partial_t v_\varepsilon(q,t)|^2\,\mathrm{d}\Sigma_0 \leq C\,\varepsilon \sup_{t\in(0,\varepsilon)} \int_{\Sigma_t} |\partial_n\psi_\varepsilon|^2\,.$$

Now, however, the situation is worse than for ϕ_0, because ψ_ε belongs only to $H^2(\Omega_\varepsilon^{0+})$, where

$$\Omega_\varepsilon^{0+} := \{\mathcal{L}(q,t) : q\in\Sigma_0,\ 0<t<\varepsilon\}\,,$$

is diminishing as $\varepsilon \to 0$. Consequently, (16.12) would give not useful ε-dependent estimate on the norm of the trace operator associated with the embedding $H^2(\Omega_\varepsilon^{0+}) \to H^1(\Sigma_t)$ with $t \in (0,\varepsilon)$. Instead, we integrate by parts

$$\begin{aligned}
\|\partial_t v_\varepsilon\|^2_{L^2(\Sigma_0\times(0,\varepsilon))} &= \int_{\Sigma_0\times(0,\varepsilon)} (\partial_t t)\,|\partial_t v_\varepsilon(q,t)|^2 \,\mathrm{d}\Sigma_0 \wedge \mathrm{d}t \\
&= -\int_{\Sigma_0\times(0,\varepsilon)} 2\,t\,\Re\left[\partial_t \bar{v}_\varepsilon(q,t)\,\partial_t^2 v_\varepsilon(q,t)\right] \mathrm{d}\Sigma_0 \wedge \mathrm{d}t \\
&\quad + \varepsilon \lim_{t\to\varepsilon^-} \int_{\Sigma_0} |\partial_t v_\varepsilon(q,t)|^2 \,\mathrm{d}\Sigma_0 \\
&\le C\,\varepsilon \left(\|\psi_\varepsilon\|^2_{H^2(\Omega_\varepsilon^{0+})} + \|\tau^-_{+\varepsilon}\partial_n\psi_\varepsilon\|^2_{L^2(\Sigma_{+\varepsilon})} \right),
\end{aligned}$$

where the inequality employs $t \le \varepsilon$ and the geometric estimates (16.21) together with $\partial_t^2 v_\varepsilon = \partial_n^2 \psi_\varepsilon \circ \mathcal{L}$. Recall that the trace operator $\tau^-_{+\varepsilon}$ is defined in (16.14). The trick is to replace $\tau^-_{+\varepsilon}\partial_n\psi_\varepsilon$ by $\tau^+_{+\varepsilon}\partial_n\psi_\varepsilon$ using the interface condition (16.15) and employ (16.12) in the other set that does not diminish as $\varepsilon \to 0$:

$$\begin{aligned}
\|\tau^-_{+\varepsilon}\partial_n\psi_\varepsilon\|_{L^2(\Sigma_{+\varepsilon})} &\le \|\tau^+_{+\varepsilon}\partial_n\psi_\varepsilon\|_{L^2(\Sigma_{+\varepsilon})} + |\alpha_+|\,\|\tau_{+\varepsilon}\psi_\varepsilon\|_{L^2(\Sigma_{+\varepsilon})} \\
&\le C\left(\|\psi_\varepsilon\|_{H^2(\Omega_\varepsilon^+)} + |\alpha_+|\,\|\psi_\varepsilon\|_{H^1(\mathbb{R}^d)} \right).
\end{aligned}$$

Using Lemma 16.3 and (16.43), we eventually get the desired bound

$$\|\partial_t v_\varepsilon\|_{L^2(\Sigma_0\times(0,\varepsilon))} \le C\sqrt{\varepsilon}\,\|\Psi\|_{L^2(\mathbb{R}^d)}.$$

Summing up, we have proved

$$|I_1| \le C\,\varepsilon\,\|\Phi\|_{L^2(\mathbb{R}^d)}\,\|\Psi\|_{L^2(\mathbb{R}^d)}. \tag{16.45}$$

This bound together with (16.44) implies

$$\left|(\phi_0,\psi_\varepsilon)_{L^2(\Sigma_0)} - (\phi_0,\psi_\varepsilon)_{L^2(\Sigma_{+\varepsilon})}\right| \le C\,\varepsilon\,\|\Phi\|_{L^2(\mathbb{R}^d)}\,\|\Psi\|_{L^2(\mathbb{R}^d)}$$

and a similar estimate holds for the other difference of boundary terms in (16.41). Consequently,

$$\left|(\Phi,[R_\varepsilon(z)-R_0(z)]\Psi)_{L^2(\mathbb{R}^d)}\right| \le C\,\varepsilon\,\|\Phi\|_{L^2(\mathbb{R}^d)}\,\|\Psi\|_{L^2(\mathbb{R}^d)},$$

which proves (16.4) for $z \in \mathbb{C}$ with $\Re z < z_0$. The extension to other values of z is standard (*cf* [21, Sec. IV.3.3]). □

Remark 16.3. Taking into account Remark 16.2, (16.41) implies the operator identity

$$R_\varepsilon(z) - R_0(z) = R_0(z)\left[(\alpha_+ + \alpha_-)\tau_0^*\tau_0 - \alpha_+\tau^*_{+\varepsilon}\tau_{+\varepsilon} - \alpha_-\tau^*_{-\varepsilon}\tau_{-\varepsilon}\right] R_\varepsilon(z), \tag{16.46}$$

where

$$\tau_t^* : L^2(\Sigma_t) \to H^{-1}(\mathbb{R}) : \{\psi \mapsto \psi\,\delta_{\Sigma_t}\}.$$

It is a generalisation of the *first resolvent identity* known for regular potentials.

16.4 Convergence of eigenvalues and eigenfunctions

In this section, we deduce from Theorem 16.1 a convergence of eigenvalues and eigenfunctions of H_ε to eigenvalues and eigenfunctions of H_0 as $\varepsilon \to 0$. In fact, it is immediately seen that the eigenfunctions converge in the topology of $L^2(\mathbb{R}^d)$. By using the maximum principle in a refined way, we show the non-trivial property that the convergence actually holds uniformly in a neighbourhood of Σ_0. This result will be needed in Section 16.5 to prove Theorem 16.2.

Let λ_0 stand for a simple eigenvalue of H_0 with the corresponding eigenfunction ψ_0 which is assumed to be normalised according to the usual requirement for non-self-adjoint spectral problems, *i.e.*,

$$\left(\overline{\psi_0},\psi_0\right)_{L^2(\mathbb{R}^d)} = \int_{\mathbb{R}^d} \psi_0^2 = 1.$$

By a simple eigenvalue we always mean that of algebraic multiplicity one. Note that $\overline{\psi_0}$ represents an eigenfunction of the adjoint operator H_0^* corresponding to the eigenvalue $\overline{\lambda_0}$. Define

$$\mathcal{C}_r := \{z \in \mathbb{C} : |z - \lambda_0| = r\}, \tag{16.47}$$

where the radius r is chosen is such a way that the circle $\mathcal{C}_r$ surrounds only one point of $\sigma_{\mathrm{disc}}(H_0)$, the discrete spectrum of H_0. The resolvent convergence proved in the previous section allows us to claim that there exists $\varepsilon_0 > 0$ such that for any non-negative $\varepsilon < \varepsilon_0$ the circle $\mathcal{C}_r$ surrounds only one point λ_ε of $\sigma_{\mathrm{disc}}(H_\varepsilon)$. Let P_ε stand for the eigenprojector

$$P_\varepsilon := \frac{i}{2\pi} \oint_{\mathcal{C}_r} R_\varepsilon(z)\,\mathrm{d}z\,, \tag{16.48}$$

where the integration path traces out the circle around in a counterclockwise manner. Let ψ_ε stand for the eigenfunction of H_ε corresponding to λ_ε and impose the same normalisation condition $\big(\overline{\psi_\varepsilon}, \psi_\varepsilon\big)_{L^2(\mathbb{R}^d)} = 1$. Then the corresponding eigenprojector takes the form

$$P_\varepsilon = \big(\overline{\psi_\varepsilon}, \cdot\big)_{L^2(\mathbb{R}^d)}\, \psi_\varepsilon\,.$$

The following statement is a simple consequence of the norm-resolvent convergence (Theorem 16.1) proved in the previous section.

Corollary 16.1. *The asymptotics*

$$\|P_\varepsilon - P_0\|_{L^2(\mathbb{R}^d)\to L^2(\mathbb{R}^d)} = O(\varepsilon) \tag{16.49}$$

holds. Consequently, we have

$$|\lambda_\varepsilon - \lambda_0| = O(\varepsilon) \qquad \textit{and} \qquad \|\psi_\varepsilon - \psi_0\|_{L^2(\mathbb{R}^d)} = O(\varepsilon)\,. \tag{16.50}$$

The rest of this section is devoted to showing that the convergence of eigenfunctions holds in a better topology, at least in a neighbourhood of Σ_0. First of all, we establish a regularity of eigenfunctions.

Proposition 16.1. *Given $\varepsilon \geq 0$, let ψ_ε denote an eigenfunction of H_ε. Then*

$$\psi_\varepsilon \in H^m\big(\mathbb{R}^d \setminus (\Sigma_{+\varepsilon} \cup \Sigma_{-\varepsilon})\big) \qquad \textit{for all} \qquad m \in \mathbb{N}\,. \tag{16.51}$$

Proof. We have $H_\varepsilon\psi_\varepsilon = \lambda_\varepsilon\psi_\varepsilon$, where $\lambda_\varepsilon \in \mathbb{C}$ is the eigenvalue and $\psi_\varepsilon \in \mathsf{D}(H_\varepsilon)$. For $m = 2$ the claim of the lemma follows from the characterisation of the operator domain (16.16). Starting from the definition of the operator H_ε through its quadratic form (16.7) defined on the Sobolev space $H^1(\mathbb{R}^d)$, the H^2-regularity outside $\Sigma_{+\varepsilon} \cup \Sigma_{-\varepsilon}$ is actually established by our Lemma 16.3. For the present eigenvalue problem, we can write

$$(H_\varepsilon - z)\psi_\varepsilon = (\lambda_\varepsilon - z)\psi_\varepsilon =: \Psi_\varepsilon\,, \tag{16.52}$$

where z is any number from the resolvent set of H_ε. Recalling that H_ε acts as the Laplacian outside $\overline{\Sigma_{+\varepsilon}\cup\Sigma_{-\varepsilon}}$, from elliptic regularity theory (see, *e.g.*, [13, Thm. 6.3.2]), we immediately get $\psi_\varepsilon \in H^m(\mathbb{R}^d \setminus \overline{\Omega^0_{a/4}})$ for all $m \in \mathbb{N}$. It remains to show the H^m-regularity close to the parallel hypersurfaces $\Sigma_{+\varepsilon} \cup \Sigma_{-\varepsilon}$.

Let us comment on the proof for $\varepsilon = 0$. The case of positive ε is proved analogously. We refer to [13, Sec. 6.3] for more details on this type of elliptic-regularity-type arguments. Setting $v := \mathcal{U}\psi_0$ and $V := \mathcal{U}\Psi_0 = (\lambda_\varepsilon - z)v$, where $\mathcal{U}$ is the unitary transform (16.24) implementing the natural curvilinear coordinates in a vicinity of Σ_0, (16.52) yields a weak formulation of the problem

$$\left\{\begin{array}{rll} (-\Delta_G - z)v = V & \text{in} & \Sigma_0 \times (-a,a)\,, \\ v(q,0^+) - v(q,0^-) = 0 & \text{on} & \Sigma_0\,, \\ \partial_t v(q,0^+) - \partial_t v(q,0^-) = (\alpha_+ + \alpha_-)v(q,0) & \text{on} & \Sigma_0\,, \end{array}\right. \tag{16.53}$$

where the Laplace-Beltrami operator $-\Delta_G$ acts as in (16.25). Once we know that the right hand side V belongs to $H^2\big(\Sigma_0 \times [(-a,0)\cup(0,a)]\big)$, we can differentiate (16.53) (in the sense of weak derivatives) and obtain that the derivative $\partial_\rho v$ with $\rho \in \{1,\dots,d-1\}$ again satisfies the same problem (16.53), including the same interface conditions, but with a changed right hand side $V' \in L^2(\Sigma_0 \times (-a/2,a/2))$. By applying Lemma 16.3, we deduce $\partial_\rho v \in H^2\big(\Sigma_0 \times [(-a/2,0)\cup(0,a/2)]\big)$. The fact that also respective restrictions of $\partial_t^3 v$ belong to $L^2(\Sigma_0 \times (0,a/2))$ and $L^2(\Sigma_0 \times (-a/2,0))$ can be then shown from the differential equation that $\partial_\rho v$ satisfies almost everywhere, by writing as in (16.39). Hence, we have established $v \in H^3\big(\Sigma_0 \times [(-a/2,0)\cup(0,a/2)]\big)$. In particular, $V' \in H^2(\Sigma_0 \times (-a/2,a/2))$. Repeating this argument, we eventually obtain $v \in H^m\big(\Sigma_0 \times [(-a/2,0)\cup(0,a/2)]\big)$ for all $m \in \mathbb{N}$. $\square$

The proposition has the usual corollary that the eigenfunctions are smooth outside the interface hypersurfaces.

Corollary 16.2. *Let ψ_ε denote an eigenfunction of H_ε. Then ψ_ε is continuous in $\mathbb{R}^d$ and*

$$\psi_\varepsilon \in \begin{cases} C^\infty(\overline{\Omega}) \cap C^\infty(\overline{\mathbb{R}^d \setminus \Omega}) & \text{if} \quad \varepsilon = 0\,, \\ C^\infty(\overline{\Omega^0_\varepsilon}) \cap C^\infty(\overline{\mathbb{R}^d \setminus \Omega^0_\varepsilon}) & \text{if} \quad \varepsilon > 0\,. \end{cases} \tag{16.54}$$

Proof. By Proposition 16.1, we have $\psi_0 \in H^m(\mathbb{R}^d \setminus \Sigma_0)$ for every positive integer m. Hence, by the Sobolev embedding theorem (see, *e.g.*, [1, Thm. 5.4]), $\psi_0 \in C^k(\overline{\Omega}) \cap C^k(\overline{\mathbb{R}^d \setminus \Omega})$ for each positive integer k. This proves (16.54) for $\varepsilon = 0$. The continuity follows from the fact that ψ_0 as an element of the form domain $\mathsf{D}(h_0)$ belongs to $H^1(\mathbb{R}^d)$. The claims for positive ε are proved analogously. □

As a consequence of this corollary, the eigenvalue problem $H_\varepsilon \psi_\varepsilon = \lambda_\varepsilon \psi_\varepsilon$ can be considered in a classical sense. Setting

$$\phi_\varepsilon := \psi_\varepsilon - \psi_0 \tag{16.55}$$

and combining the eigenvalue equations for $\varepsilon > 0$ and $\varepsilon = 0$, we see that ϕ_ε with positive ε is a continuous and piecewise smooth solution of the classical boundary value problem

$$\begin{cases} -\Delta\phi_\varepsilon - \lambda_\varepsilon \phi_\varepsilon = (\lambda_\varepsilon - \lambda_0)\psi_0 & \text{in} \quad \mathbb{R}^d \setminus (\Sigma_{+\varepsilon} \cup \Sigma_{-\varepsilon} \cup \Sigma_0)\,, \\ \tau^+_{\pm\varepsilon}\partial_n\phi_\varepsilon - \tau^-_{\pm\varepsilon}\partial_n\phi_\varepsilon - \alpha_\pm \tau_{\pm\varepsilon}\phi_\varepsilon = \alpha_\pm \tau_{\pm\varepsilon}\psi_0 & \text{on} \quad \Sigma_{\pm\varepsilon}\,, \\ \tau^+_{+0}\partial_n\phi_\varepsilon - \tau^-_{-0}\partial_n\phi_\varepsilon = -(\alpha_+ + \alpha_-)\tau_0\psi_0 & \text{on} \quad \Sigma_0\,. \end{cases} \tag{16.56}$$

To establish the uniform convergence of eigenfunctions, we use the maximum principle following the ideas of [19]. The first ingredient is a version of the mean value theorem in the present setting.

Lemma 16.4. *For every $x \in \mathbb{R}^d$ and $r > 0$, we have the identity*

$$\begin{aligned} \phi_\varepsilon(x) = {} & \frac{1}{|\partial B_r|}\int_{\partial B_r}\phi_\varepsilon \\ & + \int_0^r \frac{\mathrm{d}\rho}{|\partial B_\rho|}\Bigg[\lambda_\varepsilon \int_{B_\rho}\phi_\varepsilon - \alpha_+\int_{\Sigma^\rho_{+\varepsilon}}\phi_\varepsilon - \alpha_-\int_{\Sigma^\rho_{-\varepsilon}}\phi_\varepsilon \\ & + (\lambda_\varepsilon - \lambda_0)\int_{B_\rho}\psi_0 - \alpha_+\int_{\Sigma^\rho_{+\varepsilon}}\psi_0 - \alpha_-\int_{\Sigma^\rho_{-\varepsilon}}\psi_0 + (\alpha_+ + \alpha_-)\int_{\Sigma^\rho_0}\psi_0\Bigg]\,, \end{aligned} \tag{16.57}$$

where ϕ_ε denotes the difference of eigenfunctions (16.55)*, $B_r \equiv B_r(x)$ is the open ball of radius r centred at x, $|\partial B_r|$ stands for the $(d-1)$-dimensional Hausdorff measure of its boundary and $\Sigma^r_{\pm\varepsilon} := \Sigma_{\pm\varepsilon} \cap B_r$.*

Proof. The formula follows by integrating the differential equation of (16.56) in the ball B_ρ of radius $\rho \in (0, r]$, using the interface conditions of (16.56) after an application of the divergence theorem and handling the boundary term $\int_{\partial B_\rho} \partial\phi_\varepsilon/\partial\nu$, with ν denoting the outward unit normal to ∂B_ρ , as in the classical mean value theorem, see [20, Thm. 2.1]. □

To handle the first term on the right hand side of (16.57), we use the following elementary result ([19, Lem. 3.14]).

Lemma 16.5. *Let $\phi \in L^2(\mathbb{R}^d)$ and $\delta > 0$. For every $x \in \mathbb{R}^d$, there exists $r = r(x, \phi, \delta) \in (0, \delta]$ such that*

$$\frac{1}{|\partial B_r|}\int_{\partial B_r}|\phi| \leq \frac{1}{|B_\delta|^{1/2}}\,\|\phi\|_{L^2(B_\delta)}\,.$$

Here $|B_r|$ denotes the d-dimensional Lebesgue measure of the ball B_r.

Proof. Assume by contradiction that there exists a point $x \in \mathbb{R}^d$ such that for all $r \in (0, \delta]$ the reverse inequality holds. Then one easily arrives at a contradiction by using in addition the coarea formula and the Schwarz inequality. □

Now we are in a position to establish the uniform convergence of eigenfunctions. While Proposition 16.1 and its Corollary 16.2 deal with *any* eigenfunctions of H_ε, from now on we assume again that ψ_ε and ψ_0 are eigenfunctions of H_ε and H_0, respectively, corresponding to simple eigenvalues λ_ε and λ_0 as described in the beginning of this section.

Theorem 16.3. *We have*

$$\|\psi_\varepsilon - \psi_0\|_{L^\infty(\Sigma_{\pm\varepsilon})} = O(\varepsilon)\,. \tag{16.58}$$

Proof. Assume that $0 < \varepsilon \le \delta/2$, where $\delta < a$ is a positive number independent of ε that will be additionally restricted later on. From (16.56) and the methods of the theory of interior regularity of solutions of elliptic problems (see, *e.g.*, [13, Sec. 6.3.1]), we deduce the bound

$$\|\phi_\varepsilon\|_{H^{m+2}(\mathbb{R}^d\setminus\overline{\Omega_\delta^0})} \le C\left(\|\phi_\varepsilon\|_{L^2(\mathbb{R}^d)} + |\lambda_\varepsilon - \lambda_0|\|\psi_0\|_{H^m(\mathbb{R}^d\setminus\Sigma_0)}\right)$$

for every $m \in \mathbb{N}$. Here the constant C depends on d, δ and m, but it is independent of ε (the dependence of the coefficient λ_ε on ε on the left hand side of the differential equation in (16.56) is unimportant due to Corollary 16.1). Within this proof, the symbol C denotes a generic constant whose value may change from line to line, but it is always independent of ε. By the convergence results of Corollary 16.1, the regularity of Proposition 16.1 and the Sobolev embedding theorem, we obtain

$$\|\phi_\varepsilon\|_{C^k(\overline{\mathbb{R}^d\setminus\Omega_\delta^0})} \le C\,\varepsilon \tag{16.59}$$

for every $k \in \mathbb{N}$. In particular, this proves the uniform convergence of eigenfunctions in $\mathbb{R}^d \setminus \Omega_\delta^0$. To prove the uniform convergence in a neighbourhood of Σ_0 containing the colliding hypersurfaces $\Sigma_{+\varepsilon}$ and $\Sigma_{-\varepsilon}$, we give slightly different proofs in high and low dimensions.

$\boxed{d \ge 3}$ First of all, we employ Lemma 16.4 with $x \in \Omega_\delta^0$ and $r \le \delta$. We estimate the terms on the right hand side of (16.57) as follows. For every continuous function $\phi \in L^\infty(\mathbb{R}^d)$, we have

$$\left|\int_0^r \frac{\mathrm{d}\rho}{|\partial B_\rho|}\int_{B_\rho}\phi\right| \le \|\phi\|_{L^\infty(\Omega_{2\delta}^0)}\int_0^r \frac{|B_\rho|}{|\partial B_\rho|}\,\mathrm{d}\rho = \|\phi\|_{L^\infty(\Omega_{2\delta}^0)}\,\frac{r^2}{2d}\,,$$
$$\left|\int_0^r \frac{\mathrm{d}\rho}{|\partial B_\rho|}\int_{\Sigma_{\pm\varepsilon}^\rho}\phi\right| \le \|\phi\|_{L^\infty(\Sigma_{\pm\varepsilon})}\int_0^r \frac{|\Sigma_{\pm\varepsilon}^\rho|}{|\partial B_\rho|}\,\mathrm{d}\rho \le C\,\|\phi\|_{L^\infty(\Sigma_{\pm\varepsilon})}\,r\,.$$

Here the last estimate employs the geometric bound $|\Sigma_{\pm\varepsilon}^\rho| \le C\rho^{d-1}$. Consequently, using Corollary 16.1,

$$\begin{aligned}\left|\lambda_\varepsilon\int_0^r \frac{\mathrm{d}\rho}{|\partial B_\rho|}\int_{B_\rho}\phi_\varepsilon\right| &\le C\,\|\phi_\varepsilon\|_{L^\infty(\Omega_{2\delta}^0)}\,\delta^2\,,\\ \left|(\lambda_\varepsilon-\lambda_0)\int_0^r \frac{\mathrm{d}\rho}{|\partial B_\rho|}\int_{B_\rho}\psi_0\right| &\le C\,\varepsilon\,,\\ \left|\alpha_\pm\int_0^r \frac{\mathrm{d}\rho}{|\partial B_\rho|}\int_{\Sigma_{\pm\varepsilon}^\rho}\phi_\varepsilon\right| &\le C\,\|\phi_\varepsilon\|_{L^\infty(\Sigma_{\pm\varepsilon})}\,\delta\,.\end{aligned} \tag{16.60}$$

To handle the last terms on the right hand side of (16.57), we recall the unitary transform (16.24). Setting $v_0 := \mathcal{U}\psi_0$, we have

$$\begin{aligned}\int_{\Sigma_\varepsilon^\rho}\psi_0 - \int_{\Sigma_0^\rho}\psi_0 &= \int_{p_\varepsilon^{-1}(\Sigma_\varepsilon^\rho)} v_0(q,\varepsilon)\,f(q,\varepsilon)\,\mathrm{d}q - \int_{\Sigma_0^\rho} v_0(q,0)\,\mathrm{d}q\\ &= \int_{p_\varepsilon^{-1}(\Sigma_\varepsilon^\rho)\cap\Sigma_0^\rho}\int_0^\varepsilon \partial_t(v_0 f)(q,t)\,\mathrm{d}t\,\mathrm{d}q\\ &\quad + \int_{p_\varepsilon^{-1}(\Sigma_\varepsilon^\rho)\setminus\Sigma_0^\rho} v_0(q,\varepsilon)\,f(q,\varepsilon)\,\mathrm{d}q - \int_{\Sigma_0^\rho\setminus p_\varepsilon^{-1}(\Sigma_\varepsilon^\rho)} v_0(q,0)\,\mathrm{d}q\,,\end{aligned}$$

where $p_\varepsilon(q) := \mathcal{L}(q,\varepsilon)$. Consequently,

$$\begin{aligned}\left|\int_{\Sigma_\varepsilon^\rho}\psi_0 - \int_{\Sigma_0^\rho}\psi_0\right| &\le |\Sigma_0|\,\varepsilon\,\|v_0\|_{C^1(\overline{\Sigma_0\times(0,\delta)})}\,\|f\|_{C^1(\overline{\Sigma_0\times(0,\delta)})}\\ &\quad + \left|p_\varepsilon^{-1}(\Sigma_\varepsilon^\rho)\bigtriangleup\Sigma_0^\rho\right|\,\|v_0\|_{C^0(\overline{\Sigma_0\times(0,\delta)})}\,\|f\|_{C^0(\overline{\Sigma_0\times(0,\delta)})}\,.\end{aligned}$$

It is a matter of purely geometric considerations to check that the estimate

$$\left|p_\varepsilon^{-1}(\Sigma_\varepsilon^\rho)\bigtriangleup\Sigma_0^\rho\right| \le C\,\varepsilon^{(d-1)/2} \tag{16.61}$$

holds true. Hence, in view of (16.18) and Corollary 16.2, we get the estimate

$$\left|\int_{\Sigma_\varepsilon^\rho}\psi_0 - \int_{\Sigma_0^\rho}\psi_0\right| \le C\,\varepsilon\,. \tag{16.62}$$

The same bound holds for $\Sigma^\rho_{-\varepsilon}$ instead of Σ^ρ_ε. Summing up, using the estimates (16.60) and (16.62) in (16.57) and assuming that $\delta \leq 1$, we arrive at

$$|\phi_\varepsilon(x)| \leq \frac{1}{|\partial B_r|} \int_{\partial B_r} |\phi_\varepsilon| + C\,\varepsilon + C\,\|\phi_\varepsilon\|_{L^\infty(\Omega^0_{2\delta})}\,\delta\,. \tag{16.63}$$

Let $x_\varepsilon \in \Omega^0_\delta$ be a point in which $|\phi_\varepsilon|$ achieves its maximum in $\overline{\Omega^0_\delta}$, *i.e.* $\sup_{x\in\Omega^0_\delta} |\phi_\varepsilon(x)| = |\phi_\varepsilon(x_\varepsilon)|$. We write

$$\|\phi_\varepsilon\|_{L^\infty(\Omega^0_{2\delta})} \leq \|\phi_\varepsilon\|_{L^\infty(\Omega^0_\delta)} + \|\phi_\varepsilon\|_{L^\infty(\Omega^0_{2\delta}\setminus\Omega^0_\delta)} \leq |\phi_\varepsilon(x_\varepsilon)| + C\,\varepsilon\,,$$

where the second inequality follows from (16.59). Using this estimate in (16.63), we obtain

$$(1-C\delta)\,|\phi_\varepsilon(x_\varepsilon)| \leq \frac{1}{|\partial B_r|} \int_{\partial B_r} |\phi_\varepsilon| + C\,\varepsilon\,. \tag{16.64}$$

Consequently, choosing δ sufficiently small in comparison to the constant C on the left hand side (coming from (16.59)), we arrive at

$$\|\phi_\varepsilon\|_{L^\infty(\Omega^0_\delta)} = |\phi_\varepsilon(x_\varepsilon)| \leq \frac{C}{|\partial B_r|} \int_{\partial B_r} |\phi_\varepsilon| + C\,\varepsilon\,. \tag{16.65}$$

Finally, applying Lemma 16.5 to the right hand side of (16.65), we get

$$\|\phi_\varepsilon\|_{L^\infty(\Omega^0_\delta)} \leq \frac{C}{|B_\delta|^{1/2}}\,\|\phi_\varepsilon\|_{L^2(B_\delta)} + C\,\varepsilon\,.$$

By Corollary 16.1 and (16.59), we obtain the uniform convergence

$$\|\phi_\varepsilon\|_{L^\infty(\mathbb{R}^d)} \leq C\,\varepsilon\,, \tag{16.66}$$

which in particular implies (16.58).

$\boxed{d=2}$ The above proof fails in low dimensions, because (16.61) does not give the desired decay rate of order ε. In dimension $d=2$, however, just a slight modification is needed to repair it by noticing that the better estimate

$$\left|p_\varepsilon^{-1}(\Sigma^\rho_\varepsilon) \bigtriangleup \Sigma^\rho_0\right| \leq C\,\varepsilon^{d-1} \tag{16.67}$$

holds (in all dimensions) provided that the centre x of the ball B_r is chosen within a distance of order ε from Σ_0. More specifically, we choose $x \in \Omega^0_{2\varepsilon}$. Then (16.62) does hold even if $d=2$. At the same time, the first term in (16.60) must be handled differently; we use the Schwarz inequality to get

$$\left|\lambda_\varepsilon \int_0^r \frac{\mathrm{d}\rho}{|\partial B_\rho|} \int_{B_\rho} \phi_\varepsilon\right| \leq C\,\|\phi_\varepsilon\|_{L^\infty(\Omega^0_{2\varepsilon})} \int_0^r \frac{|B_\rho|^{1/2}}{|\partial B_\rho|}\,\mathrm{d}\rho\,, \tag{16.68}$$

where the integral on the right hand side equals $r/(2\sqrt{\pi})$. Consequently, estimate (16.63) can be replaced by

$$|\phi_\varepsilon(x)| \leq \frac{1}{|\partial B_r|} \int_{\partial B_r} |\phi_\varepsilon| + C\,\varepsilon + C\,\|\phi_\varepsilon\|_{L^\infty(\Omega^0_{2\varepsilon})}\,\delta\,. \tag{16.69}$$

Choosing now $x_\varepsilon \in \Omega^0_{2\varepsilon}$ to be a point in which $|\phi_\varepsilon|$ achieves its maximum in $\overline{\Omega^0_{2\varepsilon}}$, we again get the estimate (16.64) and applying Lemma 16.5 together with Corollary 16.1, we obtain

$$\|\phi_\varepsilon\|_{L^\infty(\Omega^0_{2\varepsilon})} \leq C\,\varepsilon\,. \tag{16.70}$$

In particular, it implies (16.58).

$\boxed{d=1}$ We do not see a way how to make the present proof work in dimension $d=1$, where even (16.67) gives just a uniform bound, so we get no decay in ε for the left hand side of (16.62). In the one-dimensional situation, however, the eigenvalue problem is explicitly solvable (see Appendix) and it can be checked by hand that the uniform convergence (16.66) holds. □

Remark 16.4. We point out that the previous proof gives the uniform convergence of eigenfunctions (16.66) in the whole $\mathbb{R}^d$ with $d \geq 3$. It holds also if $d=1$ by an explicit verification. If $d=2$, we only get (16.70) and (16.59) (these results holds in all dimensions, of course) and the global bound (16.66) with ε being replaced by $\sqrt{\varepsilon}$ on the right hand side.

As a consequence of Theorem 16.3, we get the following lemma that will be needed in the next section.

Lemma 16.6. *We have*

$$\int_{\Sigma_{\pm\varepsilon}} \psi_0\, \partial_n^{\pm}(\psi_\varepsilon - \psi_0) = O(\varepsilon)\,.$$

Proof. Let $\xi \in C_0^\infty(\Omega_a^0)$ be a real-valued function such that $\xi = 1$ on $\Omega_\varepsilon^+ \equiv \{\mathcal{L}(q,t) : q \in \Sigma_0,\, \varepsilon < t < a/2\}$, *cf* (16.13). Multiplying (16.56) by $\xi\psi_0$ and integrating by parts over the larger set $\tilde{\Omega}_\varepsilon^+ := \{\mathcal{L}(q,t) : q \in \Sigma_0,\, \varepsilon < t < a\}$, we arrive at the identity

$$-\int_{\tilde{\Omega}_\varepsilon^+} \Delta(\xi\psi_0)\,\phi_\varepsilon - \int_{\Sigma_{+\varepsilon}} \partial_n^+\psi_0\,\phi_\varepsilon + \int_{\Sigma_{+\varepsilon}} \psi_0\,\partial_n^+\phi_\varepsilon - \lambda_\varepsilon \int_{\tilde{\Omega}_\varepsilon^+} \xi\psi_0\,\phi_\varepsilon = (\lambda_\varepsilon - \lambda_0)\int_{\tilde{\Omega}_\varepsilon^+} \xi\psi_0^2\,.$$

From Corollary 16.1 and Theorem 16.3 together with Corollary 16.2, we thus deduce

$$\int_{\Sigma_{+\varepsilon}} \psi_0\,\partial_n^+\phi_\varepsilon = O(\varepsilon)\,.$$

This proves the claim for $\Sigma_{+\varepsilon}$. The other asymptotics is proved analogously. □

16.5 Eigenvalue asymptotics

This section is devoted to a proof of Theorem 16.2 and its extension to degenerate eigenvalues.

16.5.1 Simple eigenvalues

The analysis of the eigenvalue asymptotics will be based on the formula

$$\lambda_\varepsilon = \frac{h_\varepsilon\big(\overline{P_\varepsilon\psi_0}, P_\varepsilon\psi_0\big)}{\big(\overline{P_\varepsilon\psi_0}, P_\varepsilon\psi_0\big)_{L^2(\mathbb{R}^d)}}\,, \tag{16.71}$$

where

$$h_\varepsilon\big(\overline{P_\varepsilon\psi_0}, P_\varepsilon\psi_0\big) = h_0\big(\overline{\psi_0}, \psi_0\big) + (h_\varepsilon - h_0)\big(\overline{\psi_0}, \psi_0\big) - h_\varepsilon\big(\overline{P_\varepsilon^\perp\psi_0}, P_\varepsilon^\perp\psi_0\big) \tag{16.72}$$

and

$$P_\varepsilon^\perp := I - P_\varepsilon\,.$$

Note that the analogous decomposition was also a starting point for the eigenvalues analysis derived in [18] and [16]. However, our further strategy is based on essentially different arguments. In particular, it requires certain modifications to the non-self-adjoint class of operators considered in this paper.

The first term on the right hand side of (16.72) yields $h_0(\overline{\psi_0}, \psi_0) = \lambda_0$. The following statement will allow to estimate the second term.

Proposition 16.2. *Suppose $\psi \in H^1(\mathbb{R}^d) \cap C^\infty(\overline{\Omega_0^+}) \cap C^\infty(\overline{\Omega_0^-})$. Then we have*

$$h_\varepsilon(\overline{\psi}, \psi) - h_0(\overline{\psi}, \psi) = \varepsilon\left(\alpha_+ \int_{\Sigma_0} \partial_n^+\psi^2 + \alpha_- \int_{\Sigma_0} \partial_n^-\psi^2 - (\alpha_+ - \alpha_-)(d-1)\int_{\Sigma_0} K_1\,\psi^2\right) + O(\varepsilon^2)\,, \tag{16.73}$$

where the error term depends on ψ.

Proof. Similarly as above, we define $v := \mathcal{U}\psi$, which reflects the continuity properties of ψ. A straightforward calculation yields

$$\begin{aligned} h_\varepsilon(\overline{\psi}, \psi) - h_0(\overline{\psi}, \psi) = \alpha_+ &\int_{\Sigma_0} v(q,\varepsilon)^2\, f(q,\varepsilon)\,\mathrm{d}\Sigma_0 \\ &+ \alpha_- \int_{\Sigma_0} v(q,-\varepsilon)^2\, f(q,-\varepsilon)\,\mathrm{d}\Sigma_0 \\ &- (\alpha_+ + \alpha_-)\int_{\Sigma_0} v(q,0)^2\,\mathrm{d}\Sigma_0\,. \end{aligned} \tag{16.74}$$

Employing the continuity properties of v, we can expand

$$v(q,\pm\varepsilon) = v(q,0) \pm \varepsilon\, \partial_t v(q,0^\pm) + \breve{v}_\varepsilon\,,$$

where $\|\breve{v}_\varepsilon\|_{L^2(\Sigma_0)} = O(\varepsilon^2)$. Applying these asymptotics to (16.74) and combining it with (16.18), we get the sought statement. $\square$

The third term of (16.72) is estimated by means of the following lemma.

Lemma 16.7. *The asymptotics*

$$h_\varepsilon\big(\overline{P_\varepsilon^\perp \psi_0}, P_\varepsilon^\perp \psi_0\big) = \varepsilon \left((\alpha_+^2 + \alpha_-^2) \int_{\Sigma_0} \psi_0^2 \right) + O(\varepsilon^2) \tag{16.75}$$

holds, where the error term depends on ψ_0*.*

Proof. Let us denote

$$\eta_\varepsilon(z) := \frac{i}{2\pi}\big(R_\varepsilon(z) - R_0(z)\big)\psi_0\,.$$

Then

$$P_\varepsilon^\perp \psi_0 = \int_{C_r} \eta_\varepsilon(z)\,\mathrm{d}z\,.$$

A straightforward calculation yields

$$\begin{aligned}
h_\varepsilon\big(\overline{P_\varepsilon^\perp \psi_0}, P_\varepsilon^\perp \psi_0\big) &= \int_{\mathcal{C}_r} \mathrm{d}z (h_\varepsilon - z)\big(\overline{P_\varepsilon^\perp \psi_0}, \eta_\varepsilon(z)\big) + \int_{\mathcal{C}_r} \mathrm{d}z\, z (\overline{P_\varepsilon^\perp \psi_0}, \eta_\varepsilon(z))_{L^2(\mathbb{R}^d)} \\
&= \frac{i}{2\pi}(h_0 - h_\varepsilon)\big(\overline{P_\varepsilon^\perp \psi_0}, \int_{\mathcal{C}_r} \mathrm{d}z\, R_0(z)\psi_0\big) \\
&\quad + \int_{\mathcal{C}_r} \mathrm{d}z\, z\, \big(\overline{P_\varepsilon^\perp \psi_0}, \eta_\varepsilon(z)\big)_{L^2(\mathbb{R}^d)} \\
&= (h_0 - h_\varepsilon)\big(\overline{P_\varepsilon^\perp \psi_0}, \psi_0\big) + \int_{\mathcal{C}_r} \mathrm{d}z\, z\, \big(\overline{P_\varepsilon^\perp \psi_0}, \eta_\varepsilon(z)\big)_{L^2(\mathbb{R}^d)}\,,
\end{aligned} \tag{16.76}$$

where we have used the fact $\frac{i}{2\pi}\int_{\mathcal{C}_r} \mathrm{d}z\, R_0(z)\psi_0 = \psi_0$ and the equivalence

$$(h_\varepsilon - z)\,\big(u, \big(R_\varepsilon(z) - R_0(z)\big)\psi_0\big) = (h_0 - h_\varepsilon)(u, R_0(z)\psi_0) \tag{16.77}$$

valid for all $u \in H^1(\mathbb{R}^d)$ (*cf* [21, Sec. VIII.3.2]). It follows from (16.49) that

$$P_\varepsilon \psi_0 = (\overline{\psi_\varepsilon}, \psi_0)_{L^2(\mathbb{R}^d)}\psi_\varepsilon = (1 + O(\varepsilon))\psi_\varepsilon\,.$$

Moreover,

$$P_\varepsilon^\perp \psi_0 = (1 + O(\varepsilon))\psi_\varepsilon - \psi_0\,, \qquad \|P_\varepsilon^\perp \psi_0\|_{L^2(\mathbb{R}^d)} = O(\varepsilon)\,, \tag{16.78}$$

which implies

$$\big(\overline{P_\varepsilon \psi_0}, P_\varepsilon \psi_0\big)_{L^2(\mathbb{R}^d)} = 1 + O(\varepsilon^2)\,. \tag{16.79}$$

Using the above asymptotics, we conclude that the second term on the last line of (16.76) behaves as $O(\varepsilon^2)$.

It remains to estimate the first term on the last line of (16.76). Applying the notations $v_0 := \mathcal{U}\psi_0$ and $w_\varepsilon := \mathcal{U}P_\varepsilon^\perp \psi_0$, we get

$$\begin{aligned}
(h_\varepsilon - h_0)\big(\overline{P_\varepsilon^\perp \psi_0}, \psi_0\big) &= \alpha_+ \underbrace{\int_{\Sigma_0} \big((w_\varepsilon v_0)(q,\varepsilon) - (w_\varepsilon v_0)(q,0)\big)\,\mathrm{d}\Sigma_0}_{L_1^+} \\
&\quad + \alpha_- \underbrace{\int_{\Sigma_0} \big((w_\varepsilon v_0)(q,-\varepsilon) - (w_\varepsilon v_0)(q,0)\big)\,\mathrm{d}\Sigma_0}_{L_1^-} \\
&\quad + \alpha_+ \underbrace{\int_{\Sigma_0} (w_\varepsilon v_0)(q,\varepsilon)\,\big(f(q,\varepsilon) - 1\big)\,\mathrm{d}\Sigma_0}_{L_2^+} \\
&\quad + \alpha_- \underbrace{\int_{\Sigma_0} (w_\varepsilon v_0)(q,-\varepsilon)\big(f(q,-\varepsilon) - 1\big)\,\mathrm{d}\Sigma_0}_{L_2^-}\,.
\end{aligned}$$

Using again the bound (16.42) together with the Schwarz inequality, we estimate

$$|L_2^\pm| \le C\varepsilon \, \|w_\varepsilon\|_{L^2(\Sigma_{\pm\varepsilon})} \|v_0\|_{L^2(\Sigma_{\pm\varepsilon})} \,. \tag{16.80}$$

Employing now the statement of Theorem 16.3 we conclude

$$\|w_\varepsilon\|_{L^2(\Sigma_{\pm\varepsilon})} = O(\varepsilon)\,, \tag{16.81}$$

which leads to $L_2^\pm = O(\varepsilon^2)$ in view of (16.80) and the fact that $\|v_0\|_{L^2(\Sigma_{\pm\varepsilon})}$ can be uniformly bounded. This means that $L_2^\pm$ contributes to the error term.

To estimate $L_1^\pm$ we rely on the regularity of eigenfunctions established in Lemma 16.1. For $g \in \{w_\varepsilon, v_0\}$, we have the expansion

$$g(q,0) = g(q,\pm\varepsilon) \mp \varepsilon \, \partial_t g(q, \pm\varepsilon^\mp) + \breve{g}_\varepsilon \,,$$

where $\breve{g}_\varepsilon \in L^2(\Sigma_0)$ admits the norm asymptotics of type $O(\varepsilon^2)$. This implies

$$L_1^\pm = \pm\varepsilon L_3^\pm \pm \varepsilon L_4^\pm$$

with

$$L_3^\pm := \int_{\Sigma_0} (\partial_t w_\varepsilon(q, \pm\varepsilon^\mp))\, v_0(q,\pm\varepsilon) \, \mathrm{d}\Sigma_0 \,.$$

$$L_4^\pm := \int_{\Sigma_0} w_\varepsilon(q,\pm\varepsilon)\, \partial_t v_0(q,\pm\varepsilon) \, \mathrm{d}\Sigma_0 \,.$$

Note that since v_0 is smooth for $t \neq 0$, we do not need to distinguish “left” and “right” limits for $\partial_t v_0(q,\pm\varepsilon)$. Employing again (16.81) and $\|\partial_t v_0\|_{L^2(\Sigma_{\pm\varepsilon})} \le C$, we claim that $L_4^\pm = O(\varepsilon)$, *i.e.* $\varepsilon L_4^\pm$ contributes to the error term. It remains to estimate $L_3^\pm$. To this aim we use the boundary conditions which for v_ε read

$$\partial_t v_\varepsilon(q,\pm\varepsilon^+) - \partial_t v_\varepsilon(q,\pm\varepsilon^-) = \alpha_\pm v_\varepsilon(q,\pm\varepsilon)\,.$$

Using these equivalences and decomposition (16.78), we obtain

$$L_3^\pm = -\alpha_\pm \int_{\Sigma_0} (v_\varepsilon v_0)(q,\pm\epsilon)\, \mathrm{d}\Sigma_0 \\ \pm \int_{\Sigma_0} \partial_t \big(v_\varepsilon(q,\pm\varepsilon^\pm) - v_0(q,\pm\varepsilon^\mp)\big) v_0(q,\pm\varepsilon)\, \mathrm{d}\Sigma_0 + O(\varepsilon)\,.$$

Employing again $v_0(q,\pm\varepsilon^\mp) = v_0(q,\pm\varepsilon^\pm)$ and combining it with the statements of Theorem 16.3 and Lemma 16.6, we obtain

$$L_3^\pm = -\alpha_\pm \int_{\Sigma_0} v_0^2 \, \mathrm{d}\Sigma_0 + O(\varepsilon)\,.$$

Summing up, the above estimates we come to (16.75), which completes the proof. □

Now we are in a position to establish Theorem 16.2.

Proof of Theorem 16.2. Combining (16.49), (16.75), (16.79) and (16.71) we get

$$\lambda_\varepsilon = \frac{h_\varepsilon\big(\overline{P_\varepsilon\psi_0}, P_\varepsilon\psi_0\big)}{\big(\overline{P_\varepsilon\psi_0}, P_\varepsilon\psi_0\big)_{L^2(\mathbb{R}^d)}} = \lambda_0 + \varepsilon\lambda_0' + O(\varepsilon^2)\,,$$

where λ_0' is defined by (16.6). □

16.5.2 Degenerate eigenvalues

In this subsection, we extend Theorem 16.2 to the case of degenerate eigenvalues. More specifically, now we assume that λ_0 is a discrete *semisimple* eigenvalue of H_0. The semisimple property means that the algebraic multiplicity can be greater than one, but it is still equal to the geometric multiplicity of the eigenvalue (*cf* [21, Sec. I.5.3]). It is the most general situation in the self-adjoint setting (*i.e.* $\alpha_\pm \in \mathbb{R}$ in our case).

Let $k \in \mathbb{N}$ stand for the multiplicity of λ_0 and let $\{\psi_0^i\}_{i=1}^k$ denote a system of linearly independent eigenvectors of H_0, normalised in such a way that the biorthonormal relations

$$\big(\overline{\psi_0^i}, \psi_0^j\big)_{L^2(\mathbb{R}^d)} = \delta_{ij} \tag{16.82}$$

hold true for all $i,j \in \{1,\dots,k\}$. We note that $\big\{\overline{\psi_0^i}\big\}_{i=1}^k$ constitutes a system of linearly independent eigenvectors of the adjoint H_0^* corresponding to the semisimple eigenvalue $\overline{\lambda_0}$ of the same multiplicity k.

Our main result reads as follows.

Theorem 16.4. *Let λ_0 be a semisimple discrete eigenvalue of H_0 of multiplicity $k \geq 1$ and let $\{\psi_0^i\}_{i=1}^k$ stand for a system of the corresponding eigenfunctions normalised via (16.82). There exist positive constants ε_0 and r such that, for all $\varepsilon < \varepsilon_0$, H_ε possesses precisely k (counting the algebraic multiplicity) discrete eigenvalues $\{\lambda_\varepsilon^i\}_{i=1}^k$ in the open disk of radius r centred at λ_0. Moreover, $\{\lambda_\varepsilon^i\}_{i=1}^k$ admit the following asymptotics*

$$\lambda_\varepsilon^i = \lambda_0 + \lambda_i'\,\varepsilon + o(\varepsilon)\,, \tag{16.83}$$

where $\{\lambda_i'\}_{i=1}^k$ are eigenvalues (counting the algebraic multiplicity) of the matrix $S \equiv \{s_{ij}\}_{i,j=1}^k$ with entries

$$s_{ij} := \alpha_+ \int_{\Sigma_0} \partial_n^+(\psi_0^i\psi_0^j) + \alpha_- \int_{\Sigma_0} \partial_n^-(\psi_0^i\psi_0^j) - \int_{\Sigma_0} \left[\alpha_+^2 + \alpha_-^2 + (\alpha_+ - \alpha_-)\,(d-1)K_1\right] \psi_0^i\psi_0^j\,. \tag{16.84}$$

Proof. Relying again on the norm-resolvent convergence of Theorem 16.1, we can choose $r > 0$ in such a way that the circle $\mathcal{C}_r$ introduced in (16.47) surrounds k eigenvalues of H_ε for all ε small enough. These eigenvalues admit the following asymptotics

$$\lambda_\varepsilon^i = \lambda_0 + O(\varepsilon)\,, \qquad i = 1, \dots, k\,. \tag{16.85}$$

Let us denote by ψ_ε^i, $i = 1, ..., k$, the corresponding linearly independent eigenfunctions of H_ε with the normalisation $(\overline{\psi_\varepsilon^i}, \psi_\varepsilon^i)_{L^2(\mathbb{R}^d)} = 1$. Then we can find a system $\{\psi_0'^i\}_{i=1}^k$ of eigenfunctions of H_0 corresponding to λ_0 such that

$$\psi_\varepsilon^i = P_\varepsilon \psi_0'^i\,, \tag{16.86}$$

where P_ε stands for the eigenprojector onto the space spanned by $\{\psi_\varepsilon^i\}_{i=1}^k$. To show (16.86) it suffices to check that $\{P_\varepsilon\psi_0'^i\}_{i=1}^k$ forms a basis in $\mathsf{R}(P_\varepsilon)$. Using the convergence (16.49) of spectral projections defined by (16.48), we get the asymptotics

$$\|P_\varepsilon\psi_0'^i - \psi_0'^i\|_{L^2(\mathbb{R}^d)} = \|P_\varepsilon\psi_0'^i - P_0\psi_0'^i\|_{L^2(\mathbb{R}^d)} = O(\varepsilon) \tag{16.87}$$

for $i = 1, \dots, k$. Consequently,

$$\begin{aligned}\big(\overline{P_\varepsilon\psi_0'^i}, P_\varepsilon\psi_0'^j\big)_{L^2(\mathbb{R}^d)} &= \big(\overline{\psi_0'^i}, \psi_0'^j\big)_{L^2(\mathbb{R}^d)} - \big(\overline{P_\varepsilon^\perp\psi_0'^i}, P_\varepsilon^\perp\psi_0'^j\big)_{L^2(\mathbb{R}^d)}\\ &= \big(\overline{\psi_0'^i}, \psi_0'^j\big)_{L^2(\mathbb{R}^d)} + O(\varepsilon^2)\,.\end{aligned} \tag{16.88}$$

It follows from the above asymptotics that $\{P_\varepsilon\psi_0'^i\}_{i=1}^k$ forms a linearly independent system. Actually, $\{P_\varepsilon\psi_0'^i\}_{i=1}^k$ constitutes a basis of the range of P_ε, since $\dim \mathsf{R}(P_\varepsilon) = k$.

The eigenvalues λ_ε^i of H_ε are determined by the eigenvalues of the diagonal matrix

$$D := \{d_i\delta_{ij}\}_{i,j=1}^k \qquad \text{with} \qquad d_i := \big(\overline{H_\varepsilon\psi_\varepsilon^i}, \psi_\varepsilon^i\big)_{L^2(\mathbb{R}^d)} = h_\varepsilon\big(\overline{P_\varepsilon\psi_0'^i}, P_\varepsilon\psi_0'^i\big)\,.$$

Now we repeat the steps from the proof of Theorem 16.3 and show

$$\|\psi_\varepsilon^i - \psi_0'^i\|_{L^\infty(\Sigma_{\pm\varepsilon})} = O(\varepsilon)$$

for $i = 1, \dots, k$. Furthermore, we employ the decomposition

$$h_\varepsilon\big(\overline{P_\varepsilon\psi_0'^i}, P_\varepsilon\psi_0'^i\big) = h_0\big(\overline{\psi_0'^i}, \psi_0'^i\big) + (h_\varepsilon - h_0)\big(\overline{\psi_0'^i}, \psi_0'^i\big) - h_\varepsilon\big(\overline{P_\varepsilon^\perp\psi_0'^i}, P_\varepsilon^\perp\psi_0'^i\big)\,.$$

Repeating the arguments from the proofs of Proposition 16.2 and Lemma 16.7, we establish

$$\lim_{\varepsilon\to 0} \frac{h_\varepsilon\big(\overline{\psi_0'^i}, \psi_0'^i\big) - h_0\big(\overline{\psi_0'^i}, \psi_0'^i\big)}{\varepsilon} = \alpha_+ \int_{\Sigma_0} \partial_n^+(\psi_0'^i\psi_0'^i) + \alpha_- \int_{\Sigma_0} \partial_n^-(\psi_0'^i\psi_0'^i) - (\alpha_+ - \alpha_-)(d-1) \int_{\Sigma_0} K_1\,\psi_0'^i\psi_0'^i \tag{16.89}$$

and

$$h_\varepsilon\big(\overline{P_\varepsilon^\perp\psi_0'^i}, P_\varepsilon^\perp\psi_0'^i\big) = \varepsilon\,(\alpha_+ + \alpha_-) \int_{\Sigma_0} \psi_0'^i\psi_0'^i + O(\varepsilon^2)\,. \tag{16.90}$$

Since $\{\psi_0'^j\}_{j=1}^k$ is a basis, we can express any vector ψ_0^j, $j = 1, \dots, k$ satisfying biorthonormal relation (16.82), as a linear combination $\psi_0^j = \sum_{i=1}^k a_{ji}\psi_0'^i$, where $a_{ji} \in \mathbb{C}$. Furthermore, let us define matrix S' as D expressed in the new basis, precisely

$$S' := \{s_{ij}'\}_{i,j=1}^k\,, \qquad \text{with} \quad s_{ij}' = (\overline{a_i}, Da_j)_{l_k^2}\,,$$

where $a_i := (a_{i1}, \dots, a_{ik}) \in l_k^2$. The eigenvalues of S' and D coincide. Furthermore, applying (16.89) and (16.90), we conclude that $s_{ij}' = \lambda_0\delta_{ij} + s_{ij}\varepsilon + O(\varepsilon^2)$ which implies the claim. □

16.6 Appendix: Colliding quantum dots

In this appendix, we focus on the special situation of two approaching point interactions on the real line. The simplicity of the problem enables one to derive more precise asymptotic formulae by a different method. At the same time, the explicit solutions provide a valuable insight into the origin of the individual components in the first-order correction term.

16.6.1 Eigenvalue asymptotics

As a special case of (16.7), we consider the m-sectorial operator H_ε associated with the form

$$h_\varepsilon[\psi] := \int_{\mathbb{R}} |\psi'(x)|^2 \, \mathrm{d}x + \alpha_+ |\psi(\varepsilon)|^2 + \alpha_- |\psi(-\varepsilon)|^2 , \qquad \mathsf{D}(h_\varepsilon) := H^1(\mathbb{R}) .$$

Note that the functions from $H^1(\mathbb{R})$ are continuous and, in this case, the images of the trace maps are just determined by function values $\psi(\pm\varepsilon)$.

For $\varepsilon = 0$, the operator H_0 defines a well known model: one-point interaction in one dimension with the coupling constant $\alpha_+ + \alpha_-$. The spectrum of H_0 consists of the essential (in fact continuous) spectrum $[0, \infty)$ and, under the condition $\Re(\alpha_+ + \alpha_-) < 0$, one simple discrete eigenvalue

$$\lambda_0 := -\frac{(\alpha_+ + \alpha_-)^2}{4} \tag{16.91}$$

associated with the eigenfunction

$$\psi_0(x) := C_0 \, f_0(x) , \qquad f_0(x) := \mathrm{e}^{(\alpha_+ + \alpha_-)|x|/2} .$$

Here the complex constant C_0 is chosen in such a way that the standard normalisation condition for non-self-adjoint spectral problems $\int_{\mathbb{R}} \psi_0^2 = 1$ holds.

The case of two point interactions in one dimension corresponding to $\varepsilon > 0$ is also studied in the literature, at least in the self-adjoint case (see [2, Chap. II.2] and [22]). The semi-axis $[0, \infty)$ still constitutes the essential spectrum of H_ε and possible eigenvalues λ_ε equal $-\kappa_\varepsilon^2$, where κ_ε are determined as positive solutions of the implicit equation

$$(\alpha_+ + 2\kappa)(\alpha_- + 2\kappa) - \alpha_+ \alpha_- \mathrm{e}^{-4\kappa\varepsilon} = 0 . \tag{16.92}$$

For ε small enough equation (16.92) admits a unique solution κ_ε which behaves as

$$\kappa_\varepsilon = \frac{\alpha_+ + \alpha_-}{2} + \alpha_+ \alpha_- \varepsilon + O(\varepsilon^2) \tag{16.93}$$

as $\varepsilon \to 0$. The following theorem summarises the above discussion.

Theorem 16.5 ($d = 1$)**.** *Let $\Re(\alpha_+ + \alpha_-) < 0$. For ε small enough operator H_ε has a unique simple discrete eigenvalue which admits the following asymptotics*

$$\lambda_\varepsilon = \lambda_0 - (\alpha_+ + \alpha_-)\alpha_+ \alpha_- \, \varepsilon + O(\varepsilon^2) \tag{16.94}$$

or, equivalently,

$$\lambda_\varepsilon = \lambda_0 + \Big[\alpha_+ \, \psi_0^{2\,\prime}(0^+) - \alpha_- \, \psi_0^{2\,\prime}(0^-) - (\alpha_+^2 + \alpha_-^2) \, \psi_0^2(0) \Big] \, \varepsilon + O(\varepsilon^2) . \tag{16.95}$$

Proof. The first formula is due to (16.93), while its equivalent form follows by identities $\psi_0^{2\,\prime}(0^\pm) = \mp(\alpha_+ + \alpha_-)^2/2$ and $\psi_0^2(0) = -(\alpha_+ + \alpha_-)/2$. □

Note that (16.95) is a special case of the general formula (16.6).

16.6.2 More insight into the first-order correction term

The aim of this section is to discuss in more detail the first-order correction for the two-point interaction model. In particular, we would like to analyse the source of the term $-(\alpha_+^2 + \alpha_-^2)\psi_0(0)^2$.

The general solution of the eigenvalue problem $H_\varepsilon f_\varepsilon = \lambda_\varepsilon f_\varepsilon$ takes the form

$$f_\varepsilon(x) = \begin{cases} \mathrm{e}^{\kappa_\varepsilon x} & \text{for} \quad x < -\varepsilon , \\ c_1 \mathrm{e}^{-\kappa_\varepsilon x} + c_2 \mathrm{e}^{\kappa_\varepsilon x} & \text{for} \quad -\varepsilon < x < \varepsilon , \\ c_3 \mathrm{e}^{-\kappa_\varepsilon x} & \text{for} \quad x > \varepsilon . \end{cases} \tag{16.96}$$

Using the boundary conditions (16.15) at $x = \pm\varepsilon$, we determine the constants

$$c_1 = -\frac{\alpha_-}{2\kappa_\varepsilon}\,, \qquad c_2 = \frac{\alpha_- + 2\kappa_\varepsilon}{2\kappa_\varepsilon}\,, \qquad c_3 = \mathrm{e}^{2\kappa_\varepsilon\varepsilon} + \frac{\alpha_-}{2\kappa_\varepsilon}(\mathrm{e}^{2\kappa_\varepsilon\varepsilon} - \mathrm{e}^{-2\kappa_\varepsilon\varepsilon})\,. \tag{16.97}$$

Moreover, employing (16.94), we get

$$c_3 = 1 + O(\varepsilon) \tag{16.98}$$

as $\varepsilon \to 0$. Let ψ_ε stand for the normalised eigenfunction of H_ε, *i.e.*$\psi_\varepsilon := C_\varepsilon f_\varepsilon$, where the complex constant C_ε is chosen in such a way that $\int_{\mathbb{R}} \psi_\varepsilon^2 = 1$. Let P_ε denote the corresponding eigenprojector, *i.e.*

$$P_\varepsilon g := \big(\overline{\psi_\varepsilon}, g\big)_{L^2(\mathbb{R})}\ \psi_\varepsilon\,.$$

The eigenvalue λ_ε of H_ε satisfies

$$\lambda_\varepsilon = \frac{h_\varepsilon\big(\overline{P_\varepsilon\psi_0}, P_\varepsilon\psi_0\big)}{\big(\overline{P_\varepsilon\psi_0}, P_\varepsilon\psi_0\big)_{L^2(\mathbb{R})}}\,, \tag{16.99}$$

where

$$h_\varepsilon\big(\overline{P_\varepsilon\psi_0}, P_\varepsilon\psi_0\big) = h_0\big(\overline{\psi_0}, \psi_0\big) + (h_\varepsilon - h_0)\big(\overline{\psi_0}, \psi_0\big) - h_\varepsilon\big(\overline{P_\varepsilon^\perp\psi_0}, P_\varepsilon^\perp\psi_0\big) \tag{16.100}$$

with $P^\perp := I - P_\varepsilon$. The first term on the right hand side of (16.100) yields $h_0\big(\overline{\psi_0}, \psi_0\big) = \lambda_0$ since $\int_{\mathbb{R}} \psi_0^2 = 1$. The second term admits the asymptotics

$$(h_\varepsilon - h_0)\big(\overline{\psi_0}, \psi_0\big) = \Big(\alpha_+ \psi_0^{2\,\prime}(0+) - \alpha_- \psi_0^{2\,\prime}(0-)\Big)\,\varepsilon + O(\varepsilon^2)\,, \tag{16.101}$$

which reproduces the first two components of the correction term in (16.95).

The remaining discussion is devoted to the analysis of the third term on the right hand side of (16.100). A straightforward calculation using (16.97) and (16.98) yields

$$\left|\int_{\mathbb{R}} f_\varepsilon^2 - \int_{\mathbb{R}} f_0^2\right| = O(\varepsilon)\,, \qquad \|f_\varepsilon - f_0\|_{L^2(\mathbb{R})} = O(\varepsilon)\,. \tag{16.102}$$

Define

$$\omega_\varepsilon := P_\varepsilon^\perp \psi_0 = \psi_0 - \big(\overline{\psi_\varepsilon}, \psi_0\big)_{L^2(\mathbb{R})}\psi_\varepsilon\,. \tag{16.103}$$

Note that the derivative of ω_ε is well defined everywhere apart $x = 0$ and $x = \pm\varepsilon$. Let ω_ε' denote this derivative. Consequently, the third term on the right hand side of (16.100) takes the form

$$h_\varepsilon(\overline{\omega_\varepsilon}, \omega_\varepsilon) = \int_{\mathbb{R}} \omega_\varepsilon'^2 + \alpha_+\,\omega_\varepsilon^2(\varepsilon) + \alpha_-\,\omega_\varepsilon^2(-\varepsilon)\,. \tag{16.104}$$

Using again (16.97) and (16.98), we state that

$$\omega_\varepsilon(\pm\varepsilon) = O(\varepsilon)\,.$$

This means that the last two terms on the right hand side (16.104) behave as $O(\varepsilon^2)$.

Finally, let us analyse the first component (16.104). In view of (16.96), we decompose

$$\int_{\mathbb{R}} \omega_\varepsilon'^2 = \int_{-\varepsilon}^{\varepsilon} \omega_\varepsilon'^2 + \int_{-\infty}^{-\varepsilon} \omega_\varepsilon'^2 + \int_{\varepsilon}^{\infty} \omega_\varepsilon'^2\,.$$

A straightforward calculation shows that the last two terms on the right hand side behave as $O(\varepsilon^2)$. The first term requires a more detailed analysis. Namely, for $x \in (0\,, \varepsilon)$ we have

$$\omega_\varepsilon'(x) = -\frac{\alpha_+ + \alpha_-}{2}\left(-\kappa_0\mathrm{e}^{-\kappa_0 x} + c_1\kappa_\varepsilon\mathrm{e}^{-\kappa_\varepsilon x} - c_2\kappa_\varepsilon\mathrm{e}^{\kappa_\varepsilon x}\right)^2 + O(\varepsilon) = -\alpha_+ + O(\varepsilon)\,,$$

where we have used (16.97) together with the fact $\int_{\mathbb{R}} f_0^2 = -\frac{2}{\alpha_+ + \alpha_-}$. Analogously we show $\omega_\varepsilon'(x) = -\alpha_- + O(\varepsilon)$ for $x \in (-\varepsilon\,, 0)$. This implies $\int_{-\varepsilon}^{\varepsilon} \omega_\varepsilon'^2 = (\alpha_+^2 + \alpha_-^2)\varepsilon + O(\varepsilon^2)$, and consequently,

$$\int_{\mathbb{R}} \omega_\varepsilon'^2 = (\alpha_+^2 + \alpha_-^2)\varepsilon + O(\varepsilon^2)\,,$$

which, finally, leads to

$$h_\varepsilon(\overline{\omega_\varepsilon}, \omega_\varepsilon) = (\alpha_+^2 + \alpha_-^2)\varepsilon + O(\varepsilon^2)\,.$$

On the other hand,

$$(\overline{P_\varepsilon\psi_0}, P_\varepsilon\psi_0)_{L^2(\mathbb{R})} = (\overline{\psi_0}, \psi_0)_{L^2(\mathbb{R})} - (\overline{\omega_\varepsilon}, \omega_\varepsilon)_{L^2(\mathbb{R})} = 1 + O(\varepsilon^2)\,.$$

Summing up the above discussion, we have obtained the total first-order correction term in (16.95) and identified the origin of its individual terms.

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Chapter 17

Spectral stability of Schrödinger operators with subordinated complex potentials

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Spectral stability of Schrödinger operators with subordinated complex potentials

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Abstract. We prove that the spectrum of Schrödinger operators in three dimensions is purely continuous and coincides with the non-negative semiaxis for all potentials satisfying a form-subordinate smallness condition. By developing the method of multipliers, we also establish the absence of point spectrum for Schrödinger operators in all dimensions under various alternative hypotheses, still allowing complex-valued potentials with critical singularities.

17.1 Introduction

Let H_0 be the *free Hamiltonian*, *i.e.* the self-adjoint operator in $L^2(\mathbb{R}^d)$ associated with the quadratic form

$$h_0[\psi] := \int_{\mathbb{R}^d} |\nabla\psi|^2 \,, \qquad \mathsf{D}(h_0) := H^1(\mathbb{R}^d) \,.$$

Let $V : \mathbb{R}^d \to \mathbb{C}$ be a measurable function which is *form-subordinated* to H_0 with the subordination bound less than one, *i.e.*,

$$\exists a < 1 \,, \quad \forall \psi \in H^1(\mathbb{R}^d) \,, \qquad \int_{\mathbb{R}^d} |V||\psi|^2 \leq a \int_{\mathbb{R}^d} |\nabla\psi|^2 \tag{17.1}$$

In view of the criticality of H_0 in low dimensions, (17.1) is admissible for $d \geq 3$ only, to which we restrict in the sequel.

Assumption (17.1) in particular means that the quadratic form

$$v[\psi] := \int_{\mathbb{R}^d} V\,|\psi|^2 \,, \qquad \mathsf{D}(v) := \left\{ \psi \in L^2(\mathbb{R}^d) : \int_{\mathbb{R}^d} |V||\psi|^2 < \infty \right\} . \tag{17.2}$$

is relatively bounded with respect to h_0 with the relative bound less than one. Consequently, the sum $h_V := h_0 + v$ is a closed form with $\mathsf{D}(h_V) = H^1(\mathbb{R}^d)$ which gives rise to an m-sectorial operator H_V in $L^2(\mathbb{R}^d)$ via the representation theorem (*cf* [16, Thm. VI.2.1]). It is customary to write

$$H_V = H_0 \dot{+} V \,, \tag{17.3}$$

but we stress that this generalised sum in the sense of forms differs from the ordinary operator sum.

The purpose of this paper is to show that condition (17.1) is sufficient to guarantee that the spectra of H_0 and H_V coincide, at least under some extra hypotheses.

Recall that the spectrum, $\sigma(H)$, of a closed operator H in a complex Hilbert space $\mathcal{H}$ is determined by the set of points $\lambda \in \mathbb{C}$ for which $H - \lambda : \mathsf{D}(H) \to \mathcal{H}$ is not bijective. Three disjoint subsets of $\sigma(H)$ that exhaust the spectrum are distinguished: the *point spectrum* $\sigma_\mathrm{p}(H) := \{\lambda \in \mathbb{C} : H - \lambda \text{ is not injective}\}$, the *continuous spectrum* $\sigma_\mathrm{c}(H) := \{\lambda \in \sigma(H) \setminus \sigma_\mathrm{p}(H) : \overline{\mathsf{R}(H-\lambda)} = \mathcal{H}\}$ and the *residual spectrum* $\sigma_\mathrm{r}(H) := \{\lambda \in \sigma(H) \setminus \sigma_\mathrm{p}(H) : \overline{\mathsf{R}(H-\lambda)} \neq \mathcal{H}\}$.

The spectrum of H_0 is well known to be purely continuous, in fact $\sigma(H_0) = \sigma_\mathrm{c}(H_0) = [0, +\infty)$. In this paper we show that this spectral property is preserved by condition (17.1) provided that $d = 3$.

Theorem 17.1. *Let* $d = 3$ *and assume* (17.1). *Then* $\sigma(H_V) = \sigma_\mathrm{c}(H_V) = [0, +\infty)$.

The theorem is proved in four steps:

(i) Absence of the residual spectrum; Section 17.1.

(ii) Absence of the point spectrum; Section 17.2.

(iii) Absence of the continuous spectrum in $\mathbb{C} \setminus [0, +\infty)$; Section 17.3.

(iv) Inclusion of $[0,+\infty)$ in the spectrum; Section 17.4.

Property (i) follows at once (in any dimension): Since the adjoint operator satisfies $H_V^* = H_{\overline{V}} = \mathcal{T} H_V \mathcal{T}$, where $\mathcal{T}$ is the complex-conjugation operator defined by $\mathcal{T}\psi := \overline{\psi}$, H_V is $\mathcal{T}$*-self-adjoint* (*cf* [8, Sec. III.5]) and as such it has no residual spectrum (*cf* [3]). The absence of eigenvalues (ii) is established in Section 17.2 by means of an argument reminiscent of the Birman-Schwinger principle, but we emphasise that positive eigenvalues are excluded as well. Property (iii) is proved by a modified version of the previous argument in Section 17.3. Finally, in Section 17.4, we establish (iv) with help of an abstract quadratic-form criterion for the inclusion of points in the spectrum.

The present paper is primarily motivated by a recent interest in spectral theory of Schrödinger operators with complex potential, see [1, 12, 4, 19, 6, 21, 11, 7, 9, 13]. However, the role of hypothesis (17.1) to have the conclusion of Theorem 17.1 seems to be new in the self-adjoint case, too.

As a matter of fact, Simon established the absence of eigenvalues in the self-adjoint case for $d = 3$ already in [22, Thm. III.12] (see also [20, Thm. XIII.21]) by assuming

$$\|V\|_R^2 := \iint_{\mathbb{R}^3\times\mathbb{R}^3} \frac{|V(x)||V(y)|}{|x-y|^2}\, dx\, dy < (4\pi)^2 \,. \tag{17.4}$$

The extension of his method to complex potentials is straightforward. However, notice that our assumption (17.1) is weaker. Indeed, (17.1) is equivalent to (17.25), while

$$\big\||V|^{1/2} H_0^{-1/2}\big\|^2 = \big\||V|^{1/2} H_0^{-1} |V|^{1/2}\big\| \le \big\||V|^{1/2} H_0^{-1} |V|^{1/2}\big\|_{\mathrm{HS}} = \frac{\|V\|_R}{4\pi}\,, \tag{17.5}$$

where $\|\cdot\|$ and $\|\cdot\|_{\mathrm{HS}}$ denote the operator and Hilbert-Schmidt norms in $L^2(\mathbb{R}^3)$, respectively. The last equality in (17.5) follows with help of the explicit formula for the Green function (17.23) in $\mathbb{R}^3$.

To be more specific, notice that, by virtue of the *classical Hardy inequality*

$$\forall \psi \in H^1(\mathbb{R}^d)\,, \qquad \int_{\mathbb{R}^d} |\nabla\psi|^2 \ge \left(\frac{d-2}{2}\right)^2 \int_{\mathbb{R}^d} \frac{|\psi(x)|^2}{|x|^2}\, dx\,, \tag{17.6}$$

our hypothesis (17.1) is in particular satisfied for potentials V verifying

$$|V(x)| \le a \left(\frac{d-2}{2}\right)^2 \frac{1}{|x|^2} \tag{17.7}$$

for almost every $x \in \mathbb{R}^d$. However, the Hardy potential on the right hand side of this inequality does not even belong to the Rollnik class characterised for $d = 3$ by the norm $\|\cdot\|_R$ in (17.4). Furthermore, the location of the continuous spectrum without the hypothesis that V belongs to the Rollnik class (which ensures the finiteness of the Hilbert-Schmidt norm above) is less evident in our more general setting.

Our Theorem 17.1 is also an improvement upon the non-self-adjoint situation considered by Frank in [11, Thm. 2]. First, he establishes the absence of eigenvalues outside $[0,+\infty)$ only. Second, his assumption to get the conclusion of Theorem 17.1 for $d = 3$ is

$$\int_{\mathbb{R}^3} |V(x)|^{3/2}\, dx < \frac{3^{3/2}}{4\pi^2}\,, \tag{17.8}$$

which is again stronger than ours (17.1). Indeed, by the Hölder and Sobolev inequalities,

$$\int_{\mathbb{R}^3} |V||\psi|^2 \le \left(\int_{\mathbb{R}^3} |V|^{3/2}\right)^{2/3} \left(\int_{\mathbb{R}^3} |\psi|^6\right)^{1/3} \le \left(\int_{\mathbb{R}^3} |V|^{3/2}\right)^{2/3} \frac{2^{4/3}}{3\pi^{4/3}} \int_{\mathbb{R}^3} |\nabla\psi|^2\,, \tag{17.9}$$

for all $\psi \in H^1(\mathbb{R}^3)$. As an example, the Hardy potential on the right hand side of (17.7) makes the left hand side of (17.8) infinite, while it is an admissible potential for our Theorem 17.1. Finally, let us mention that Frank and Simon have noticed recently in [13] that even positive eigenvalues can be excluded.

Our hypothesis (17.1) is of course intrinsically a smallness condition about V. But it is interesting to notice that it involves potentials with quite rough local singularities, *e.g.* (17.7). It seems that such potentials are not typically covered by previous works on the exclusion of embedded eigenvalues, even in the self-adjoint case; see [15, 17] to quote just the most recent results based on Carleman's estimates.

The extension of Theorem 17.1 to higher dimensions is not obvious, since our method relies on the pointwise inequality for Green's functions (17.27), which does not hold for $d > 3$. As an alternative approach, in Section 17.5, we develop the technique of multipliers for Schrödinger operators with complex-valued potentials and prove the absence of eigenvalues in any dimension under a stronger hypothesis.

Theorem 17.2. *Let $d \geq 3$ and assume*

$$\exists b < \frac{d-2}{5d-8}\,, \quad \forall \psi \in H^1(\mathbb{R}^d)\,, \qquad \int_{\mathbb{R}^d} r^2\,|V|^2\,|\psi|^2 \leq b^2 \int_{\mathbb{R}^d} |\nabla\psi|^2\,, \tag{17.10}$$

where $r(x) := |x|$. Then $\sigma_{\mathrm{p}}(H_V) = \varnothing$.

Notice that (17.1) follows as a consequence of (17.10) by means of the Schwarz inequality and the classical Hardy inequality (17.6). Indeed, (17.10) and (17.6) yield

$$\int_{\mathbb{R}^d} |V||\psi|^2 \leq \|rV\psi\| \left\|\frac{\psi}{r}\right\| \leq \frac{2b}{d-2} \int_{\mathbb{R}^d} |\nabla\psi|^2\,. \tag{17.11}$$

for all $\psi \in H^1(\mathbb{R}^d)$, and $b < (d-2)/2$ due to the restriction in (17.10).

Both (17.1) and (17.10) are smallness assumptions about V. Our next step is to look for some alternative conditions which guarantee the absence of eigenvalues for H_V, in all dimensions $d \geq 3$. The idea is to modify the proof of Theorem 17.2 by splitting the real and imaginary parts of the potential V and treating them separately. In order to include potentials which are not necessarily subordinated in the spirit of (17.1), we consider the space

$$\mathcal{D}(\mathbb{R}^d) := \overline{C_0^\infty(\mathbb{R}^d)}^{|||\cdot|||}\,, \qquad |||\psi|||^2 := \int_{\mathbb{R}^d} |\nabla\psi|^2 + \int_{\mathbb{R}^d} (\Re V)_+\,|\psi|^2 + \int_{\mathbb{R}^d} |\psi|^2\,, \tag{17.12}$$

where we have introduced the notation $f_\pm := \max\{\pm f, 0\}$ for any measurable function $f : \mathbb{R}^d \to \mathbb{R}$. Clearly, $\mathcal{D}(\mathbb{R}^d)$ is continuously embedded in $H^1(\mathbb{R}^d)$ and it coincides with the latter as a set if (17.1) holds. The form $h_V^{(1)}[\psi] := \int_{\mathbb{R}^d} |\nabla\psi|^2 + \int_{\mathbb{R}^d} (\Re V)_+\,|\psi|^2$, $\mathsf{D}(h_V^{(1)}) := \mathcal{D}(\mathbb{R}^d)$, is closed by definition. Assuming now only that $(\Re V)_-$ and $\Im V$ are form-subordinated to H_0 with the subordination bound less than one (*cf* (17.14) and (17.16) below), the sum $h_V := h_V^{(1)} + h_V^{(2)}$ with $h_V^{(2)}[\psi] := -\int_{\mathbb{R}^d} (\Re V)_-\,|\psi|^2 + \int_{\mathbb{R}^d} \Im V\,|\psi|^2$ is a closed form with $\mathsf{D}(h_V) = \mathcal{D}(\mathbb{R}^d)$. Of course, h_V coincides with the previously defined form under the hypothesis (17.1). In this more general setting, we also denote by H_V the m-sectorial operator associated with h_V.

Now we are in a position to state the main result about the absence of eigenvalues for H_V under natural conditions on V.

Theorem 17.3. *Let $d \geq 3$ and assume that there exist non-negative numbers b_1, b_2, b_3 satisfying*

$$b_1^2 < 1 - \frac{2b_3}{d-2}\,, \qquad b_2^2 + 2\,b_3 + \frac{1}{4}\sqrt{b_3}\left(\frac{2}{d-2}\right)^{\frac{3}{2}} < 1\,, \tag{17.13}$$

such that, for all $\psi \in \mathcal{D}(\mathbb{R}^d)$,

$$\int_{\mathbb{R}^d} (\Re V)_-\,|\psi|^2 \leq b_1^2 \int_{\mathbb{R}^d} |\nabla\psi|^2\,, \tag{17.14}$$

$$\int_{\mathbb{R}^d} [\partial_r(r\,\Re V)]_+\,|\psi|^2 \leq b_2^2 \int_{\mathbb{R}^d} |\nabla\psi|^2\,, \tag{17.15}$$

$$\int_{\mathbb{R}^d} r^2\,|\Im V|^2\,|\psi|^2 \leq b_3^2 \int_{\mathbb{R}^d} |\nabla\psi|^2\,, \tag{17.16}$$

where $\partial_r f(x) := \frac{x}{|x|} \cdot \nabla f(x)$. Then $\sigma_{\mathrm{p}}(H_V) = \varnothing$.

We recall that (17.14) and (17.16) ensure that $h_V^{(2)}$ is subordinated to $h_V^{(1)}$ with the subordination bound less than one, so H_V is indeed well defined. A brief comparison between Theorems 17.1, 17.2 and 17.3 is in order:

- If $\Im V = 0$, namely V is real-valued, then b_3 can be chosen to be equal to zero and condition (17.13) then reads $b_1 < 1$, $b_2 < 1$. In this case, the subordination assumption (17.1) implies (17.14). However, we stress that conditions (17.14) and (17.15) are not unsigned, contrary to the case of (17.1). In particular, a large class of *repulsive* potentials such as the Coulomb-type interaction $V(x) = c\,|x|^{-1}$ with any $c > 0$ satisfy (17.14) and (17.15), although the subordination (17.1) fails.
- On the other hand, if $\Re V = 0$, namely V is purely imaginary-valued, then (17.14), (17.15) are fulfilled and one just needs to assume (17.16) with

$$\sqrt{b_3} < 8\left[\left(\frac{2}{d-2}\right)^{\frac{3}{2}} + \sqrt{\left(\frac{2}{d-2}\right)^3 + 128}\,\right]^{-1}.$$

This hypothesis is better than condition (17.10) of Theorem 17.2 and represents a completely new result, to our knowledge. However, for general complex-valued potentials V, the interest of Theorem 17.2 consists in that it requires no conditions on the derivatives of V.

The techniques used to prove Theorems 17.2 and 17.3 permit to handle more general lower-order perturbations of H_0. It is of particular interest for the *electromagnetic Hamiltonian* $H_{A,V}$ that we introduce as follows. Given a *magnetic potential* $A \in L^2_{\mathrm{loc}}(\mathbb{R}^d;\mathbb{R}^d)$ and denoting by $\nabla_A := \nabla + iA$ the magnetic gradient, we now consider the space

$$\mathcal{D}_A(\mathbb{R}^d) := \overline{C_0^\infty(\mathbb{R}^d)}^{|||\cdot|||_A}, \qquad |||\psi|||_A^2 := \int_{\mathbb{R}^d} |\nabla_A\psi|^2 + \int_{\mathbb{R}^d} (\Re V)_+\,|\psi|^2 + \int_{\mathbb{R}^d} |\psi|^2, \tag{17.17}$$

and introduce the form $h_{A,V}[\psi] := \int_{\mathbb{R}^d} |\nabla_A\psi|^2 + \int_{\mathbb{R}^d} V|\psi|^2$, $\mathsf{D}(h_{A,V}) := \mathcal{D}_A(\mathbb{R}^d)$. If V is such that (17.19) and (17.21) below hold, then $h_{A,V}$ is closed. We denote by $H_{A,V}$ the m-sectorial operator associated with $h_{A,V}$. We next denote by $B := \nabla A - (\nabla A)^t \in \mathcal{M}_{d\times d}(\mathbb{R})$ the *magnetic field* generated by A. (For $d = 3$, B may be identified with $\operatorname{curl} A$, in the sense that $Bv = v \times \operatorname{curl} A$ for all $v \in \mathbb{R}^3$, where the cross denotes the vectorial product.) Following a notation introduced in [10], we also define

$$B_\tau(x) := \frac{x}{|x|} \cdot B(x)\,. \tag{17.18}$$

(A non-trivial example of magnetic field with $B_\tau = 0$ is given in dimension $d = 3$ by the magnetic potential $A(x) = |x|^{-2}(-x_2, x_1, 0)$.)

The last result of this manuscript is an analogue of Theorem 17.3 in the presence of an external magnetic field.

Theorem 17.4. *Let $d \geq 3$, $A \in L^2_{\mathrm{loc}}(\mathbb{R}^d;\mathbb{R}^d)$ and assume that there exist non-negative numbers b_1, b_2, b_3 satisfying* (17.13) *such that, for all $\psi \in \mathcal{D}_A(\mathbb{R}^d)$,*

$$\int_{\mathbb{R}^d} (\Re V)_-\,|\psi|^2 \leq b_1^2 \int_{\mathbb{R}^d} |\nabla_A\psi|^2\,, \tag{17.19}$$

$$\int_{\mathbb{R}^d} [\partial_r(r\,\Re V)]_+\,|\psi|^2 \leq b_2^2 \int_{\mathbb{R}^d} |\nabla_A\psi|^2\,, \tag{17.20}$$

$$2\int_{\mathbb{R}^d} r^2\left(|\Im V|^2 + |B_\tau|^2\right)|\psi|^2 \leq b_3^2 \int_{\mathbb{R}^d} |\nabla_A\psi|^2\,. \tag{17.21}$$

Then $\sigma_{\mathrm{p}}(H_{A,V}) = \varnothing$.

17.2 Absence of eigenvalues: the Birman-Schwinger principle

The main role in our proof of Theorem 17.1 is played by the Birman-Schwinger operator

$$K_z := |V|^{1/2}\,(H_0 - z)^{-1}\,V_{1/2} \qquad \text{with} \qquad V_{1/2} := |V|^{1/2}\,\operatorname{sgn}(V)\,,$$

where $\operatorname{sgn}(z)$ is the complex signum function defined by $\operatorname{sgn}(z) := z/|z|$ for $z \in \mathbb{C}\setminus\{0\}$ and $\operatorname{sgn}(0) := 0$. We abuse the notation by using the same symbols for maximal operators of multiplication and their generating functions. The operator K_z is well defined (on its natural domain of the composition of three operators) for all $z \in \mathbb{C}$ and $d \geq 3$.

If $z \notin [0, +\infty)$, however, we have a useful formula for the integral kernel of K_z:

$$K_z(x,y) = |V|^{1/2}(x)\,G_z(x,y)\,V_{1/2}(y)\,, \tag{17.22}$$

where G_z is the *Green's function* of $H_0 - z$, *i.e.* the integral kernel of the resolvent $(H_0 - z)^{-1}$. We observe that K_z is a bounded operator for all $z \notin [0, +\infty)$ and $d \geq 3$ under our hypothesis (17.1). Indeed, $V_{1/2}$ maps $L^2(\mathbb{R}^d)$ to $H^{-1}(\mathbb{R}^d)$ by duality, $(H_0 - z)^{-1}$ is an isomorphism between $H^{-1}(\mathbb{R}^d)$ and $H^1(\mathbb{R}^d)$ and the latter space is mapped by $|V|^{1/2}$ back to $L^2(\mathbb{R}^d)$.

Moreover, if $d = 3$, we have an explicit formula

$$G_z(x,y) := \frac{1}{4\pi}\,\frac{e^{-\sqrt{-z}\,|x-y|}}{|x-y|}\,. \tag{17.23}$$

Here and in the sequel we choose the principal branch of the square root. Using this explicit formula, we are able to show that K_z is bounded by a under the hypothesis (17.1).

Lemma 17.1. *Let $d = 3$ and assume* (17.1). *Then*

$$\forall z \notin (0, +\infty)\,, \qquad \|K_z\| \le a\,. \tag{17.24}$$

Proof. We start with an equivalent formulation of (17.1), in any dimension $d \ge 3$. Writing $g := H_0^{1/2}\psi$ in (17.1), we have

$$\big\||V|^{1/2} H_0^{-1/2} g\big\|^2 \le a \,\big\|\nabla H_0^{-1/2} g\big\|^2 = a\,\|g\|^2\,,$$

where $\|\cdot\|$ denotes the norm in $L^2(\mathbb{R}^d)$. Since the range of $H_0^{1/2}$ is dense in $L^2(\mathbb{R}^d)$, we see that (17.1) is equivalent to

$$\big\||V|^{1/2} H_0^{-1/2}\big\|^2 \le a\,. \tag{17.25}$$

It follows (by taking the adjoint) that also

$$\big\|H_0^{-1/2}|V|^{1/2}\big\|^2 \le a\,. \tag{17.26}$$

Now we assume $d = 3$, where the explicit formula (17.23) for the Green function is available. By virtue of the pointwise bound

$$\forall z \notin (0, +\infty)\,, \quad \forall x, y \in \mathbb{R}^3\,, \qquad |G_z(x,y)| \le G_0(x,y)\,, \tag{17.27}$$

we have

$$|(f, K_z g)| \le (|f|, \tilde{K}_0 |g|) \le \|\tilde{K}_0\| \|f\| \|g\| \tag{17.28}$$

for every $z \notin (0, +\infty)$ and all $f, g \in L^2(\mathbb{R}^3)$, where

$$\tilde{K}_0 := |V|^{1/2} H_0^{-1} |V|^{1/2}$$

and $(\cdot,\cdot)$ denotes the inner product in $L^2(\mathbb{R}^3)$ (conjugate linear in the first argument). Using (17.25) and (17.26), we have

$$\|\tilde{K}_0\| = \big\||V|^{1/2} H_0^{-1} |V|^{1/2}\big\| \le \big\||V|^{1/2} H_0^{-1/2}\big\| \big\|H_0^{-1/2} |V|^{1/2}\big\| \le a\,. \tag{17.29}$$

Consequently, (17.28) and (17.29) imply (17.24). □

The following lemma provides an (integral) criterion for the existence of solutions to the (differential) eigenvalue equation of H_V. It can be considered as a one-sided version of the Birman-Schwinger principle extended to possible eigenvalues in $[0, +\infty)$ as well.

Lemma 17.2. *Let $d = 3$ and assume* (17.1). *If $H_V\psi = \lambda\psi$ with some $\lambda \in \mathbb{C}$ and $\psi \in \mathsf{D}(H_V)$, then $\phi := |V|^{1/2}\psi$ obeys*

$$\forall \varphi \in L^2(\mathbb{R}^3)\,, \qquad \lim_{\varepsilon \to 0^\pm} (\varphi, K_{\lambda + i\varepsilon}\phi) = -(\varphi, \phi)\,. \tag{17.30}$$

Proof. Given any $\lambda \in \mathbb{C}$, there is $\varepsilon_0 > 0$ such that $\lambda + i\varepsilon \notin [0, +\infty)$ for all real ε satisfying $0 < |\varepsilon| < \varepsilon_0$. By density of $C_0^\infty(\mathbb{R}^3)$ in $L^2(\mathbb{R}^3)$ and Lemma 17.1, it is enough to prove (17.30) for $\varphi \in C_0^\infty(\mathbb{R}^3)$. We have

$$(\varphi, K_{\lambda+i\varepsilon}\phi) = \iint_{\mathbb{R}^3 \times \mathbb{R}^3} \overline{\varphi(x)}\, |V|^{1/2}(x)\, G_{\lambda+i\varepsilon}(x,y)\, V(y)\, \psi(y)\, dx\, dy = \int_{\mathbb{R}^3} \eta_\varepsilon(y)\, V(y)\, \psi(y)\, dy\,, \tag{17.31}$$

where

$$\eta_\varepsilon := \int_{\mathbb{R}^3} \overline{\varphi(x)}\, |V|^{1/2}(x)\, G_{\lambda+i\varepsilon}(x, \cdot)\, dx = (H_0 - \lambda - i\varepsilon)^{-1}\, |V|^{1/2}\, \overline{\varphi}\,,$$

where the second equality holds due to the symmetry $G_z(x,y) = G_z(y,x)$. In view of (17.1), $|V|^{1/2}\overline{\varphi} \in L^2(\mathbb{R}^3)$. Since $\varepsilon \ne 0$ is so small that $\lambda + i\varepsilon \notin \sigma(H_0)$, we have $\eta_\varepsilon \in \mathsf{D}(H_0) = H^2(\mathbb{R}^3)$. In particular, $\eta_\varepsilon \in H^1(\mathbb{R}^3)$ and the weak formulation of the eigenvalue equation $H_V\psi = \lambda\psi$ yields

$$\begin{aligned}
\int_{\mathbb{R}^3} \eta_\varepsilon(y)\, V(y)\, \psi(y)\, dy &= -(\nabla\overline{\eta_\varepsilon}, \nabla\psi) + \lambda\, (\overline{\eta_\varepsilon}, \psi) \\
&= -(\nabla\overline{\psi}, \nabla\eta_\varepsilon) + \lambda\, (\overline{\psi}, \eta_\varepsilon) \\
&= -(\nabla\overline{\psi}, \nabla\eta_\varepsilon) + (\lambda + i\varepsilon)\, (\overline{\psi}, \eta_\varepsilon) - i\varepsilon\, (\overline{\psi}, \eta_\varepsilon) \\
&= -(\overline{\psi}, |V|^{1/2}\overline{\varphi}) - i\varepsilon\, (\overline{\psi}, \eta_\varepsilon) \\
&= -(\varphi, |V|^{1/2}\psi) - i\varepsilon\, (\overline{\eta_\varepsilon}, \psi)\,.
\end{aligned} \tag{17.32}$$

Here the last but one equality follows from the weak formulation of the resolvent equation $(H_0 - \lambda - i\varepsilon)\eta_\varepsilon = |V|^{1/2}\overline{\varphi}$. Consequently, (17.31) and (17.32) imply (17.30) after taking the limit $\varepsilon \to 0^\pm$, provided that $\varepsilon\,(\bar{\eta}_\varepsilon, \psi) \to 0$ as $\varepsilon \to 0$. To see the latter, we write

$$|(\overline{\eta_\varepsilon}, \psi)| = |(\varphi, M_\varepsilon \psi)| \leq \|\varphi\|\,\|M_\varepsilon\|\,\|\psi\|\,,$$

where $M_\varepsilon := \chi_\Omega\,|V|^{1/2}(H_0 - \lambda - i\varepsilon)^{-1}$ with $\Omega := \operatorname{supp}\varphi$, and it remains to show that $\varepsilon\,\|M_\varepsilon\|$ tends to zero as $\varepsilon \to 0$. Following [22, Thm. III.6], we use the resolvent kernel (17.23) and estimate $\|M_\varepsilon\| \leq \|M_\varepsilon\|_{\mathrm{HS}}$. We have

$$\|M_\varepsilon\|_{\mathrm{HS}}^2 = \frac{1}{(4\pi)^2} \iint_{\Omega\times\mathbb{R}^3} |V(x)|\, \frac{e^{-2\,\kappa(\varepsilon)\,|x-y|}}{|x-y|^2}\, dx\, dy = \frac{1}{4\pi\kappa(\varepsilon)} \int_\Omega |V(x)|\, dx\,,$$

where the last integral is bounded because $V \in L^1_{\mathrm{loc}}(\mathbb{R}^3)$ as a consequence of (17.1) and

$$\kappa(\varepsilon) := \Re\sqrt{-(\lambda + i\varepsilon)} \sim \begin{cases} |\varepsilon|^{1/2} & \text{if} \quad \lambda = 0\,, \\ |\varepsilon| & \text{if} \quad \Re\lambda > 0 \;\&\; \Im\lambda = 0\,, \\ 1 & \text{otherwise}\,. \end{cases}$$

Hence, $\varepsilon\,\|M_\varepsilon\|$ behaves at least as $\mathcal{O}(\varepsilon^{1/2})$ as $\varepsilon \to 0$, which concludes the proof of the lemma. □

Remark 17.1. Lemma 17.2 resembles [22, Thm. III.6] in the self-adjoint case. It is also related to the recent abstract result [13, Prop. 3.1].

Now we are in a position to establish the absence of eigenvalues in three dimensions.

Theorem 17.5. *Let* $d = 3$ *and assume* (17.1). *Then* $\sigma_{\mathrm{p}}(H_V) = \varnothing$.

Proof. Assume there exists $\lambda \in \mathbb{C}$ and a non-trivial $\psi \in \mathsf{D}(H_V)$ such that $H_V\psi = \lambda\psi$. Since the spectrum of H_0 is purely continuous, the theorem clearly holds for $V = 0$ and we may thus suppose that V is non-trivial. But then $\phi := |V|^{1/2}\psi$ is also non-trivial, otherwise ψ would be a non-trivial solution of $H_0\psi = \lambda\psi$, which is again impossible by the absence of eigenvalues for H_0. Now, Lemma 17.2 with $\varphi := \phi$ and Lemma 17.1 yield

$$a\,\|\phi\|^2 \geq \lim_{\varepsilon\to 0^\pm} |(\phi, K_{\lambda+i\varepsilon}\phi)| = \|\phi\|^2\,. \tag{17.33}$$

This is a contradiction because $a < 1$. □

17.3 Absence of the continuous spectrum outside $[0, +\infty)$

The following lemma is a modification of the idea behind Lemma 17.2 to deal with the continuous spectrum. We prove it in all dimensions $d \geq 3$.

Lemma 17.3. *Let* $d \geq 3$ *and assume* (17.1). *If* $\|H_V\psi_n - \lambda\psi_n\| \to 0$ *as* $n \to \infty$ *with some* $\lambda \in \mathbb{C}\setminus\mathbb{R}$ *and* $\{\psi_n\}_{n\in\mathbb{N}} \subset \mathsf{D}(H_V)$ *such that* $\|\psi_n\| = 1$ *for all* $n \in \mathbb{N}$, *then* $\phi_n := |V|^{1/2}\psi_n$ *obeys*

$$\lim_{n\to\infty} \frac{(\phi_n, K_\lambda\phi_n)}{\|\phi_n\|^2} = -1\,. \tag{17.34}$$

Proof. The proof is similar to that of Lemma 17.2. We have

$$(\phi_n, K_\lambda\phi_n) = \int_{\mathbb{R}^d} \eta_n(y)\, V(y)\, \psi_n(y)\, dy = v(\overline{\eta_n}, \psi_n)\,, \tag{17.35}$$

where $(\cdot,\cdot)$ denotes the inner product in $L^2(\mathbb{R}^d)$ and the function

$$\eta_n := \int_{\mathbb{R}^d} \overline{\phi_n(x)}\, |V|^{1/2}(x)\, G_\lambda(x,\cdot)\, dx = (H_0 - \lambda)^{-1}\, |V|^{1/2}\, \overline{\phi_n}$$

belongs to $H^1(\mathbb{R}^d)$. Indeed,

$$\eta_n = (H_0 - \lambda)^{-1}\, H_0^{1/2} H_0^{-1/2}\, |V|^{1/2}\, \overline{\phi_n}\,, \tag{17.36}$$

where $\phi_n \in L^2(\mathbb{R}^d)$ by (17.1), $H_0^{-1/2}|V|^{1/2}$ is bounded due to (17.26) and $(H_0-\lambda)^{-1}H_0^{1/2}$ maps $L^2(\mathbb{R}^d)$ to $H^1(\mathbb{R}^d)$. More specifically,

$$\|\eta_n\| \leq C_\lambda\,\sqrt{a}\,\|\phi_n\|\,, \qquad \text{where} \qquad C_\lambda := \sup_{\xi\in[0,\infty)} \left|\frac{\xi}{\xi^2 - \lambda}\right|\,. \tag{17.37}$$

In analogy with (17.32), we are thus allowed to write

$$\begin{aligned} v(\overline{\eta_n},\psi_n) &= h_V(\overline{\eta_n},\psi_n) - \lambda\,(\overline{\eta_n},\psi_n) - (\nabla\overline{\eta_n},\nabla\psi_n) + \lambda\,(\overline{\eta_n},\psi_n) \\ &= \big(\overline{\eta_n},(H_V-\lambda)\psi_n\big) - h_0(\overline{\psi_n},\eta_n) + \lambda\,(\overline{\psi_n},\eta_n)\,. \end{aligned} \tag{17.38}$$

By the second representation theorem (*cf* [16, Thm. VI.2.23]) and (17.36),

$$\begin{aligned} h_0(\overline{\psi_n},\eta_n) - \lambda\,(\overline{\psi_n},\eta_n) &= \big(H_0^{1/2}\overline{\psi_n},H_0^{1/2}\eta_n\big) - \lambda\,(\overline{\psi_n},\eta_n) \\ &= \big(H_0^{1/2}\overline{\psi_n},(H_0-\lambda+\lambda)(H_0-\lambda)^{-1}H_0^{-1/2}|V|^{1/2}\overline{\phi_n}\big) - \lambda\,(\overline{\psi_n},\eta_n) \\ &= \big(H_0^{1/2}\overline{\psi_n},H_0^{-1/2}|V|^{1/2}\overline{\phi_n}\big) \\ &= \big((H_0^{-1/2}|V|^{1/2})^*H_0^{1/2}\overline{\psi_n},\overline{\phi_n}\big) \\ &= \big(|V|^{1/2}\overline{\psi_n},\overline{\phi_n}\big) \\ &= \|\phi_n\|^2\,. \end{aligned} \tag{17.39}$$

Since

$$\|H_V\psi_n-\lambda\psi_n\| = \sup_{\substack{\varphi\in L^2(\mathbb{R}^d)\\ \varphi\neq 0}} \frac{|(\varphi,H_V\psi_n-\lambda\psi_n)|}{\|\varphi\|} \geq \big|\|\nabla\psi_n\|^2+v[\psi_n]-\lambda\big|\,,$$

where the inequality is obtained by choosing $\varphi:=\psi_n$, and the left hand side vanishes as $n\to\infty$, we see that $\Im v[\psi_n]$ tends to $\Im\lambda\neq 0$ as $n\to\infty$. In particular,

$$\liminf_{n\to\infty}\|\phi_n\|>0\,. \tag{17.40}$$

Using (17.39) in (17.38), recalling (17.35), dividing the obtained identity by $\|\phi_n\|^2$ (which is non-zero for all sufficiently large n due to (17.40)) and taking the limit as $n\to\infty$, we arrive at

$$\lim_{n\to\infty}\frac{(\phi_n,K_\lambda\phi_n)}{\|\phi_n\|^2}+1 = \lim_{n\to\infty}\frac{\big(\overline{\eta_n},(H_V-\lambda)\psi_n\big)}{\|\phi_n\|^2}\,.$$

In view of (17.37) and (17.40), the right hand side equals zero by the hypothesis. □

Now we are in a position to establish the absence of the continuous spectrum outside $[0,+\infty)$.

Theorem 17.6. *Let $d=3$ and assume* (17.1). *Then $\sigma_c(H_V)\subset[0,+\infty)$.*

Proof. By (17.1), $\Re h_V[\psi]\geq(1-a)\|\nabla\psi\|^2\geq 0$ for all $\psi\in H^1(\mathbb{R}^3)$. Since H_V is m-sectorial, it follows that the spectrum of H_V is contained in the right complex half-plane (*cf* [16, Thm. V.3.2]). Assume that there exists $\lambda\in\mathbb{C}$ with $\Re\lambda\geq 0$ and $\Im\lambda\neq 0$ such that $\lambda\in\sigma_c(H_V)$. Then λ belongs to the kind of essential spectrum which is characterised by the existence of a singular sequence of H_V corresponding to λ (*cf* [8, Thm. IX.1.3]): $\exists\{\psi_n\}_{n\in\mathbb{N}}\subset\mathsf{D}(H_V)$, $\|\psi_n\|=1$ for all $n\in\mathbb{N}$, $\|(H_V-\lambda)\psi_n\|\to 0$ as $n\to\infty$ and $\{\psi_n\}_{n\in\mathbb{N}}$ is weakly converging to zero. By Lemma 17.3 and Lemma 17.1,

$$a\geq\|K_\lambda\|\geq\left|\lim_{n\to\infty}\frac{(\phi_n,K_\lambda\phi_n)}{\|\phi_n\|^2}\right|=1\,,$$

This is a contradiction because $a<1$. □

We remark that the last step of the proof of Theorem 17.6 requires Lemma 17.1 for which $d=3$ is crucial.

17.4 Inclusion of the spectrum in $[0,+\infty)$

The opposite inclusion follows by an explicit construction of a singular sequence of H_V corresponding to non-negative energies. Since the operator H_V is defined through its sesquilinear form, it is convenient to have a criterion which requires that the singular sequence is in the form domain only. Unable to find a reference in the general case, we state the abstract version first (for the self-adjoint situation, see [18, Thm. 5]).

Lemma 17.4. *Let H be an m-sectorial accretive operator in a complex Hilbert space $\mathcal{H}$ which is associated with a (densely defined, closed, sectorial) sesquilinear form h. Given $\lambda\in\mathbb{C}$, assume that there exists a sequence $\{\phi_n\}_{n\in\mathbb{N}}\subset\mathsf{D}(h)$ such that $\|\phi_n\|=1$ for all $n\in\mathbb{N}$ and*

$$\sup_{\substack{\psi\in\mathsf{D}(h)\\ \psi\neq 0}}\frac{|h(\phi_n,\psi)-\lambda\,(\phi_n,\psi)|}{\|\psi\|_{\mathsf{D}(h)}}\xrightarrow[n\to\infty]{}0\,, \tag{17.41}$$

where $\|\psi\|_{\mathsf{D}(h)}:=\sqrt{\Re h[\psi]+\|\psi\|^2}$. Then $\lambda\in\sigma(H)$.

Remark 17.2. Notice that the left hand side of (17.41) is the norm of the vector $H^*\phi_n - \overline{\lambda}\,\phi_n$ in the dual space $\mathsf{D}(h)^*$, when $\mathsf{D}(h)$ is thought as the subspace of $\mathcal{H}$ equipped with the norm $\|\cdot\|_{\mathsf{D}(h)}$.

Proof. We proceed by contradiction: Assume the hypotheses of the theorem and $\lambda \notin \sigma(H)$. The latter means that for every $g \in \mathcal{H}$ there exists $\psi \in \mathsf{D}(H)$ such that $H\psi - \lambda\psi = g$. That is, $\psi = (H-\lambda)^{-1}g$ and $(H-\lambda)^{-1}$ is bounded as an operator on $\mathcal{H}$ onto $\mathcal{H}$. The weak formulation of the resolvent equation reads

$$\forall \phi \in \mathsf{D}(h)\,, \qquad h(\phi,\psi) - \lambda\,(\phi,\psi) = (\phi, g)\,. \tag{17.42}$$

Consequently, for every $\phi \in \mathsf{D}(h)$,

$$C_\lambda \sup_{\substack{\psi\in\mathsf{D}(h)\\ \psi\neq 0}} \frac{|h(\phi,\psi)-\lambda\,(\phi,\psi)|}{\|\psi\|_{\mathsf{D}(h)}} \geq \sup_{\substack{g\in\mathcal{H}\\ g\neq 0}} \frac{|h(\phi,\psi)-\lambda\,(\phi,\psi)|}{\|g\|} = \sup_{\substack{g\in\mathcal{H}\\ g\neq 0}} \frac{|(\phi,g)|}{\|g\|} = \|\phi\|\,, \tag{17.43}$$

where ψ and g are related through (17.42) and the constant

$$C_\lambda := \sup_{\substack{g\in\mathcal{H}\\ g\neq 0}} \frac{\|\psi\|_{\mathsf{D}(h)}}{\|g\|}$$

is finite because the resolvent $(H-\lambda)^{-1}$ maps $\mathcal{H}$ onto $\mathsf{D}(H) \subset \mathsf{D}(h)$. More specifically,

$$\begin{aligned}
\|\psi\|^2_{\mathsf{D}(h)} &= \Re h[(H-\lambda)^{-1}g] + \|(H-\lambda)^{-1}g\|^2 \\
&= \Re\big((H-\lambda)^{-1}g, H(H-\lambda)^{-1}g\big) + \|(H-\lambda)^{-1}g\|^2 \\
&\leq \big(\|(H-\lambda)^{-1}\|\|H(H-\lambda)^{-1}\| + \|(H-\lambda)^{-1}\|^2\big)\,\|g\|^2\,.
\end{aligned}$$

Choosing $\phi := \phi_n$ in (17.43), we get that the left hand side tends to zero as $n\to\infty$ by (17.41), while the right hand side equals one due to the normalisation of $\{\phi_n\}_{n\in\mathbb{N}}$, a contradiction. □

Now we are in a position to prove the inclusion of the interval $[0,+\infty)$ in the spectrum of H_V. The following result holds in all dimensions $d \geq 3$.

Theorem 17.7. *Let $d \geq 3$ and assume* (17.1). *Then $\sigma(H_V) \supset [0,+\infty)$.*

Proof. We construct the sequence $\{\phi_n\}_{n\in\mathbb{N}}$ from Lemma 17.4 applied to H_V by setting

$$\phi_n(x) := \varphi_n(x)\,e^{ik\cdot x}\,,$$

where $k \in \mathbb{R}^d$ is such that $|k|^2 = \lambda \in [0,+\infty)$, $\varphi_n(x) := n^{-d/2}\varphi_1(x/n)$ for all $n \in \mathbb{N}$ (with the convention $0 \notin \mathbb{N}$) and $\varphi_1 \in C_0^\infty(\mathbb{R}^d)$ is a function such that $\|\varphi_1\| = 1$. The normalisation factor in the definition of φ_n is chosen in such a way that

$$\|\varphi_n\| = \|\varphi_1\| = 1\,, \qquad \|\nabla\varphi_n\| = n^{-1}\,\|\nabla\varphi_1\|\,, \qquad \|\Delta\varphi_n\| = n^{-2}\,\|\Delta\varphi_1\|$$

for all $n \in \mathbb{N}$. Then $\|\phi_n\| = 1$ and $\phi_n \in \mathsf{D}(h_V) = \mathsf{D}(h_0) = H^1(\mathbb{R}^d)$ for all $n \in \mathbb{N}$. Furthermore,

$$\|-\Delta\phi_n - \lambda\,\phi_n\| = \|-\Delta\varphi_n + 2ik\cdot\nabla\varphi_n\| \leq \|\Delta\varphi_n\| + 2\,|k|\,\|\nabla\varphi_n\| \xrightarrow[n\to\infty]{} 0\,. \tag{17.44}$$

In fact, $\{\phi_n\}_{n\in\mathbb{N}}$ is the usual singular sequence of H_0 corresponding to λ. At the same time,

$$\big|v[\phi_n]\big| \leq \big\||V|^{1/2}\varphi_n\big\|^2 \leq a\,\|\nabla\varphi_n\|^2 \xrightarrow[n\to\infty]{} 0\,, \tag{17.45}$$

where the second inequality follows by (17.1).

The numerator in (17.41) can be estimated as follows

$$\begin{aligned}
|h_V(\phi_n,\psi) - \lambda\,(\phi_n,\psi)| &= |(-\Delta\phi_n - \lambda\phi_n,\psi) + v(\phi_n,\psi)| \\
&\leq \|-\Delta\phi_n - \lambda\,\phi_n\|\,\|\psi\| + \sqrt{|v[\phi_n]|}\sqrt{|v[\psi]|} \\
&\leq \|-\Delta\phi_n - \lambda\,\phi_n\|\,\|\psi\| + \sqrt{|v[\phi_n]|}\,\sqrt{a}\,\|\nabla\psi\|\,,
\end{aligned}$$

where the last inequality is due to (17.1). As for the denominator in (17.41), employing (17.1) again, we have

$$\|\psi\|^2_{\mathsf{D}(h)} = \|\nabla\psi\|^2 + \Re v[\psi] + \|\psi\|^2 \geq (1-a)\,\|\nabla\psi\|^2 + \|\psi\|^2 \geq (1-a)\,\|\psi\|^2_{\mathsf{D}(h_0)}\,,$$

where $\|\cdot\|_{\mathsf{D}(h_0)}$ is just the usual norm of $H^1(\mathbb{R}^d)$. Putting these estimates together, we have the bound

$$\sup_{\substack{\psi\in\mathsf{D}(h_V)\\ \psi\neq 0}} \frac{|h_V(\phi_n,\psi)-\lambda\,(\phi_n,\psi)|}{\|\psi\|_{\mathsf{D}(h_V)}} \leq \frac{\|-\Delta\phi_n-\lambda\phi_n\|+\sqrt{|v[\phi_n]|}\,\sqrt{a}}{\sqrt{1-a}}\,,$$

where the right hand side tends to zero due to (17.44) and (17.45).

Summing up, given $\lambda\in[0,+\infty)$, we have shown that the sequence $\{\phi_n\}_{n\in\mathbb{N}}$ satisfies all the hypotheses of Lemma 17.4. Consequently, $[0,+\infty)\subset\sigma(H_V)$. □

Proof of Theorem 17.1. To conclude, Theorem 17.1 follows as a consequence of Theorems 17.5, 17.6, 17.7 and the absence of the residual spectrum justified already in Section 17.1. □

17.5 Absence of eigenvalues: the method of multipliers

In this last section, we prove Theorems 17.2, 17.3 and 17.4 by a completely different approach in comparison with the previous sections. Namely, we extend the method of multipliers developed in the self-adjoint context in [2] to complex-valued potentials. Here we proceed in all dimensions $d\geq 3$.

Let us consider the equation

$$\Delta u+\lambda u=f, \tag{17.46}$$

where λ is any complex constant; we write $\lambda_1:=\Re\lambda$ and $\lambda_2:=\Im\lambda$. Given a measurable function $f:\mathbb{R}^d\to\mathbb{C}$ that we assume to merely belong to $H^{-1}(\mathbb{R}^d)$, we say that u is a *solution* of (17.46) if $u\in H^1(\mathbb{R}^d)$ and

$$\forall v\in H^1(\mathbb{R}^d)\,,\qquad -(\nabla v,\nabla u)+\lambda\,(v,u)=(v,f)\,. \tag{17.47}$$

Here, with an abuse of notation, the same symbol $(\cdot,\cdot)$ is used for the inner product in $L^2(\mathbb{R}^d)$ and for the duality pairing between $H^1(\mathbb{R}^d)$ and $H^{-1}(\mathbb{R}^d)$ on the left and right hand side of (17.47), respectively. Equation (17.46) is related to the eigenvalue problem of H_V by setting $f:=Vu$. Notice that any eigenvalue λ of H_V necessarily satisfies $\lambda_1>0$ due to (17.1). If u is a solution of (17.46), we set

$$u^{\pm}(x):=e^{\pm i\,\mathrm{sgn}(\lambda_2)\,\lambda_1^{\frac12}|x|}\,u(x)\,,\qquad \mathrm{sgn}(\lambda_2):=\begin{cases}\frac{\lambda_2}{|\lambda_2|} & \text{if}\quad \lambda_2\neq 0\,,\\ 1 & \text{if}\quad \lambda_2=0\,.\end{cases} \tag{17.48}$$

In order to prove Theorem 17.2, we establish the following result, which shows that (17.46) has no non-trivial solutions provided that f is small in a suitable sense.

Theorem 17.8. *Let $d\geq 3$. Let u be a solution of* (17.46) *with $\Re\lambda>0$, and assume that f satisfies*

$$\|xf\|\leq\Lambda\,\|\nabla u^-\|\,,\qquad \|xf\|\leq\Lambda\,\|\nabla u\|\,, \tag{17.49}$$

where Λ is determined by

$$\frac{2(2d-3)}{d-2}\,\Lambda+\frac{\sqrt{2}}{\sqrt{d-2}}\,\Lambda^{\frac32}<1\,. \tag{17.50}$$

Then $u=0$.

Proof. The proof relies on direct techniques, based on multiplication and integration by parts, inspired by [2], in which the methods by [5, 14] are developed and refined. Here we propose some slight modifications in the arguments, essentially due to the fact that we need to handle complex-valued potentials. To save space, we abbreviate $\int:=\int_{\mathbb{R}^d}$ and omit arguments of integrated functions.

Following [2], we divide the proof into two cases: $|\lambda_2|\leq\lambda_1$ and $|\lambda_2|>\lambda_1$.

$\boxed{\textbf{Case } |\lambda_2|\leq\lambda_1.}$ Our first step consists in approximating solutions of (17.47) by a standard cutoff and mollification argument, which is fundamental to make rigorous the proof in the sequel. To this aim, let $\xi_R:\mathbb{R}^d\to[0,1]$ be a smooth function such that

$$\xi=1 \text{ in } B_R\,,\qquad \xi=0 \text{ in } \mathbb{R}^d\setminus B_{2R}\,,\qquad |\nabla\xi_R|\leq 2R^{-1}\,,\qquad |\Delta\xi_R|\leq 2R^{-1}|x|^{-1}\,, \tag{17.51}$$

for any $R>0$ sufficiently large, where $B_R:=\{|x|<R\}$. For a function $g:\mathbb{R}^d\to\mathbb{C}$, we then denote $g_R:=g\,\xi_R$. If $u\in H^1(\mathbb{R}^d)$ is a solution to (17.47), we see that $u_R\in H^1(\mathbb{R}^d)$ solves

$$\Delta u_R+\lambda u_R=f_R-2\nabla\xi_R\cdot\nabla u-u\Delta\xi_R=:\widetilde{f}_R \tag{17.52}$$

in the weak sense of (17.47). Notice that, since f satisfies conditions (17.49) and (17.50), we have

$$\|x\widetilde{f}_R\| \le \Lambda \left\|\nabla u_R^-\right\| + \epsilon^2(R)\,, \qquad \|x\widetilde{f}_R\| \le \Lambda \left\|\nabla u_R\right\| + \epsilon^2(R)\,, \qquad \lim_{R\to\infty} \epsilon^2(R) = 0\,. \tag{17.53}$$

Indeed, by (17.51),

$$\|x\widetilde{f}_R\| \le \|xf_R\| + 8\left(\int_{R<|x|<2R} |\nabla u|^2\right)^{\frac{1}{2}} + 4R^{-2}\left(\int_{R<|x|<2R} |u|^2\right)^{\frac{1}{2}},$$

where the last two terms tends to 0 as $R \to \infty$, since $u \in H^1(\mathbb{R}^d)$.

Let now $\phi \in C_0^\infty(\mathbb{R}^d)$ be a function such that $\int \phi = 1$, and define, for any $\delta > 0$, $\phi_\delta(x) := \delta^{-d}\phi\left(\frac{x}{\delta}\right)$. If $u \in H^1(\mathbb{R}^d)$ is a solution to (17.47), we see that $u_{R,\delta} := u_R * \phi_\delta$ solves

$$\Delta u_{R,\delta} + \lambda\, u_{R,\delta} = \widetilde{f}_{R,\delta}$$

in the weak sense of (17.47), where $\widetilde{f}_{R,\delta} := \widetilde{f}_R * \phi_\delta$. More specifically,

$$\forall v \in H^1(\mathbb{R}^d)\,, \qquad (-\nabla v, \nabla u_{R,\delta}) + \lambda\,(v, u_{R,\delta}) = \left(v, \widetilde{f}_{R,\delta}\right). \tag{17.54}$$

By (17.53), it turns out that

$$\|x\widetilde{f}_{R,\delta}\| \le \Lambda \left\|\nabla u_{R,\delta}^-\right\| + \epsilon^2(R)\,, \qquad \|x\widetilde{f}_{R,\delta}\| \le \Lambda \left\|\nabla u_{R,\delta}\right\| + \epsilon^2(R)\,, \qquad \lim_{R\to\infty} \epsilon^2(R) = 0\,, \tag{17.55}$$

where $u_{R,\delta}^- := u_R^- * \phi_\delta$ and Λ as in (17.50).

We can now start with suitable algebraic manipulations of equation (17.54), which suitably approximates (17.47). Let $G_1, G_2, G_3 : \mathbb{R}^d \to \mathbb{R}$ be three smooth functions. Choosing $v := G_1 u_{R,\delta}$ in (17.54), taking the real part of the resulting identity and integrating by parts, we arrive at the identity

$$\lambda_1 \int G_1 |u_{R,\delta}|^2 - \int G_1 |\nabla u_{R,\delta}|^2 + \frac{1}{2}\int \Delta G_1\, |u_{R,\delta}|^2 = \Re \int \widetilde{f}_{R,\delta}\, G_1\, \overline{u_{R,\delta}}\,. \tag{17.56}$$

Analogously, choosing $v := G_2 u$ in (17.47) and taking the imaginary part of the resulting identity, we obtain

$$\lambda_2 \int G_2 |u_{R,\delta}|^2 - \Im \int \nabla G_2 \cdot \overline{u_{R,\delta}} \nabla u_{R,\delta} = \Im \int \widetilde{f}_{R,\delta}\, G_2\, \overline{u_{R,\delta}}\,, \tag{17.57}$$

where the dot denotes the scalar product in $\mathbb{R}^d$. Finally, choosing $v := 2\nabla G_3 \cdot \nabla u_{R,\delta} + \Delta G_3\, u_{R,\delta}$ in (17.47), taking the real part of the resulting identity and integrating by parts, we get

$$\begin{aligned} &\int \nabla u_{R,\delta} \cdot \nabla^2 G_3 \cdot \nabla \overline{u_{R,\delta}} - \frac{1}{4}\int \Delta^2 G_3\, |u_{R,\delta}|^2 + \lambda_2\, \Im \int \nabla G_3 \cdot u_{R,\delta} \nabla \overline{u_{R,\delta}} \\ &\quad = -\frac{1}{2}\Re \int \widetilde{f}_{R,\delta}\, \Delta G_3\, \overline{u_{R,\delta}} - \Re \int \widetilde{f}_{R,\delta}\, \nabla G_3 \cdot \nabla \overline{u_{R,\delta}}\,, \end{aligned} \tag{17.58}$$

where $\nabla^2 G_3$ denotes the Hessian matrix of G_3 and $\Delta^2 := \Delta\Delta$ is the bi-Laplacian. Notice that identities (17.56), (17.57), (17.58) are justified, since $u_{R,\delta} \in C_0^\infty(\mathbb{R}^d)$ and G_1, G_2, G_3 are smooth, therefore bounded, together with their derivatives of any order, inside the support of $u_{R,\delta}$.

In the following, we assume that G_1, G_2, G_3 are radial, *i.e.* there exist smooth functions $g_1, g_2, g_3 : [0,\infty) \to \mathbb{R}$ such that $G_i(x) = g_i(|x|)$ for all $x \in \mathbb{R}^d$ and $i \in \{1,2,3\}$. Then

$$\nabla G_i(x) = g_i'(|x|)\frac{x}{|x|}\,, \quad \Delta G_i(x) = g_i''(|x|) + g_i'(|x|)\frac{d-1}{|x|}\,, \quad \nabla^2 G_i(x) = g_i''(|x|)\frac{xx}{|x|^2} + \frac{g_i'(|x|)}{|x|}\left(I - \frac{xx}{|x|^2}\right),$$

where I denotes the identity on $\mathbb{R}^d$ and xx is the dyadic product of x and x. For any $g : \mathbb{R}^d \to \mathbb{C}$, denote by

$$\partial_r g(x) := \frac{x}{|x|} \cdot \nabla g(x) \qquad \text{and} \qquad \nabla_\tau g(x) := \left(I - \frac{xx}{|x|^2}\right) \cdot \nabla g(x)$$

the radial derivative and the angular gradient of g, respectively, so that $|\nabla g|^2 = |\partial_r g|^2 + |\nabla_\tau g|^2$.

Taking the sum (17.56) + $\lambda_1^{\frac{1}{2}}$(17.57) + (17.58), we obtain

$$\int |\partial_r u_{R,\delta}|^2 (g_3'' - g_1) + \int |\nabla_\tau u_{R,\delta}|^2 \left(\frac{g_3'}{|x|} - g_1\right) + \int |u_{R,\delta}|^2 \left(\lambda_1 g_1 + \lambda_2 \lambda_1^{\frac{1}{2}} g_2\right)$$
$$+ \int |u_{R,\delta}|^2 \left(\frac{1}{2}\Delta G_1 - \frac{1}{4}\Delta^2 G_3\right) - \lambda_1^{\frac{1}{2}} \Im \int \overline{u_{R,\delta}} \nabla u_{R,\delta} \cdot \nabla G_2 + \lambda_2 \Im \int u_{R,\delta}\, \nabla \overline{u_{R,\delta}} \cdot \nabla G_3$$
$$= \Re \int \widetilde{f}_{R,\delta}\, G_1\, \overline{u_{R,\delta}} + \lambda^{\frac{1}{2}} \Im \int \widetilde{f}_{R,\delta}\, G_2\, \overline{u_{R,\delta}} - \frac{1}{2} \Re \int \widetilde{f}_{R,\delta}\, \overline{u_{R,\delta}}\, \Delta G_3 - \Re \int \widetilde{f}_{R,\delta}\, \nabla \overline{u_{R,\delta}} \cdot \nabla G_3 \,. \tag{17.59}$$

Choosing $g_1 := \frac{1}{2} g_3''$ and $g_2 := \operatorname{sgn}(\lambda_2)\, g_3'$, the last identity becomes

$$\frac{1}{2} \int g_3'' \left(|\partial_r u_{R,\delta}|^2 + \lambda_1 |u_{R,\delta}|^2\right) - \operatorname{sgn}(\lambda_2)\, \lambda_1^{\frac{1}{2}} \Im \int g_3''\, \overline{u_{R,\delta}}\, \partial_r u_{R,\delta} + \int |\nabla_\tau u_{R,\delta}|^2 \left(\frac{g_3'}{r} - \frac{g_3''}{2}\right)$$
$$+ \frac{1}{4} \int |u_{R,\delta}|^2 \left(\Delta G_3'' - \Delta^2 G_3\right) + |\lambda_2|\, \lambda_1^{\frac{1}{2}} \int g_3' \, |u_{R,\delta}|^2 + \lambda_2 \Im \int g_3'\, u_{R,\delta}\, \partial_r \overline{u_{R,\delta}}$$
$$= \frac{1}{2} \Re \int \widetilde{f}_{R,\delta}\, g_3''\, \overline{u_{R,\delta}} + \lambda_1^{\frac{1}{2}} \operatorname{sgn}(\lambda_2) \Im \int \widetilde{f}_{R,\delta}\, g_3'\, \overline{u_{R,\delta}} - \frac{1}{2} \Re \int \widetilde{f}_{R,\delta}\, \overline{u_{R,\delta}}\, \Delta G_3 - \Re \int \widetilde{f}_{R,\delta}\, \nabla \overline{u_{R,\delta}} \cdot \nabla G_3 \,,$$

where $G_3''(x) := g_3''(|x|)$. Choosing now $G_3(x) := |x|^2$, the tangential and radial derivatives of u sum up and we obtain

$$\int \left(|\nabla u_{R,\delta}|^2 + \lambda_1 |u_{R,\delta}|^2\right) - 2 \operatorname{sgn}(\lambda_2)\, \lambda_1^{\frac{1}{2}} \Im \int \overline{u_{R,\delta}}\, \partial_r u_{R,\delta} + 2\, |\lambda_2|\, \lambda_1^{\frac{1}{2}} \int |x| |u_{R,\delta}|^2 + 2\lambda_2 \Im \int |x|\, u_{R,\delta}\, \partial_r \overline{u_{R,\delta}}$$
$$= (1-d) \Re \int \widetilde{f}_{R,\delta}\, \overline{u_{R,\delta}} + 2\lambda_1^{\frac{1}{2}} \operatorname{sgn}(\lambda_2) \Im \int \widetilde{f}_{R,\delta}\, |x|\, \overline{u_{R,\delta}} - 2 \Re \int \widetilde{f}_{R,\delta}\, x \cdot \nabla \overline{u_{R,\delta}} \,. \tag{17.60}$$

Using

$$|\nabla u_{R,\delta}^-|^2 = \left|\nabla u_{R,\delta} - i \operatorname{sgn}(\lambda_2)\, \lambda_1^{\frac{1}{2}} \frac{x}{|x|} u_{R,\delta}\right|^2 = |\nabla u_{R,\delta}|^2 + \lambda_1 |u_{R,\delta}|^2 - 2 \operatorname{sgn}(\lambda_2) \lambda_1^{\frac{1}{2}} \Im \left(\overline{u_{R,\delta}}\, \partial_r u_{R,\delta}\right) , \tag{17.61}$$

we can rewrite (17.60) as follows:

$$\int |\nabla u_{R,\delta}^-|^2 + 2\, |\lambda_2|\, \lambda_1^{\frac{1}{2}} \int |x| |u_{R,\delta}|^2 + 2\lambda_2 \Im \int |x|\, u_{R,\delta}\, \partial_r \overline{u_{R,\delta}}$$
$$= (1-d) \Re \int \widetilde{f}_{R,\delta}\, \overline{u_{R,\delta}} + 2\lambda_1^{\frac{1}{2}} \operatorname{sgn}(\lambda_2) \Im \int \widetilde{f}_{R,\delta}\, |x|\, \overline{u_{R,\delta}} - 2\Re \int \widetilde{f}_{R,\delta}\, x \cdot \nabla \overline{u}_{R,\delta} \,.$$

Subtracting from the last identity equation (17.56) with the choice $G_1(x) := |\lambda_2|\, \lambda_1^{-\frac{1}{2}} |x|$, we arrive at

$$\int |\nabla u_{R,\delta}^-|^2 - \frac{(d-1)}{2}\, |\lambda_2|\, \lambda_1^{-\frac{1}{2}} \int \frac{|u_{R,\delta}|^2}{|x|} + |\lambda_2|\, \lambda_1^{\frac{1}{2}} \int |x| |u_{R,\delta}|^2$$
$$+ |\lambda_2|\, \lambda_1^{-\frac{1}{2}} \int |x| |\nabla u_{R,\delta}|^2 + 2\lambda_2 \Im \int |x|\, u_{R,\delta}\, \partial_r \overline{u_{R,\delta}}$$
$$= (1-d) \Re \int \widetilde{f}_{R,\delta}\, \overline{u}_{R,\delta} + 2\lambda_1^{\frac{1}{2}} \operatorname{sgn}(\lambda_2) \Im \int \widetilde{f}_{R,\delta}\, |x|\, \overline{u_{R,\delta}} - 2 \Re \int \widetilde{f}_{R,\delta}\, x \cdot \nabla \overline{u_{R,\delta}} - |\lambda_2|\, \lambda_1^{-\frac{1}{2}} \Re \int \widetilde{f}_{R,\delta}\, |x|\, \overline{u_{R,\delta}} \,.$$

Using (17.61) again, we obtain the key identity

$$I := \int \left|\nabla u_{R,\delta}^-\right|^2 + \frac{|\lambda_2|}{\lambda_1^{\frac{1}{2}}} \int |x| \left|\nabla u_{R,\delta}^-\right|^2 - \frac{(d-1)}{2} \frac{|\lambda_2|}{\lambda_1^{\frac{1}{2}}} \int \frac{|u_{R,\delta}|^2}{|x|}$$
$$= \underbrace{(1-d) \Re \int \widetilde{f}_{R,\delta}\, \overline{u_{R,\delta}}}_{I_1} \underbrace{-2 \Re \int |x|\, \widetilde{f}_{R,\delta} \left(\partial_r \overline{u_{R,\delta}} + i \operatorname{sgn}(\lambda_2) \lambda_1^{\frac{1}{2}} \overline{u_{R,\delta}}\right)}_{I_2} \underbrace{- \frac{|\lambda_2|}{\lambda_1^{\frac{1}{2}}} \Re \int |x|\, \widetilde{f}_{R,\delta}\, \overline{u_{R,\delta}}}_{I_3} \,. \tag{17.62}$$

By the weighted Hardy inequality

$$\forall \psi \in C_0^\infty(\mathbb{R}^d)\,, \qquad \int \frac{|\psi|^2}{|x|} \le \frac{4}{(d-1)^2} \int |x| |\nabla \psi|^2 \,, \tag{17.63}$$

and the facts that $u_{R,\delta} \in C_0^\infty(\mathbb{R}^d)$ and $|u_{R,\delta}| = |u_{R,\delta}^-|$, we easily bound the left hand side of (17.62) from below by a positive quantity as follows

$$I \geq \int \left|\nabla u_{R,\delta}^-\right|^2 + \frac{|\lambda_2|}{\lambda_1^{\frac{1}{2}}} \frac{d-3}{d-1} \int |x||\nabla u_{R,\delta}^-|^2 \,. \tag{17.64}$$

We proceed by estimating the individual terms on the right hand side of (17.62) by means of $\|\nabla u_{R,\delta}^-\|^2$. By the Schwarz inequality, the Hardy inequality (17.6) and thanks to (17.55), we have

$$|I_1| \leq (d-1)\,\|x\widetilde{f}_{R,\delta}\| \left\|\frac{u_{R,\delta}}{|x|}\right\| = (d-1)\,\|x\widetilde{f}_{R,\delta}\| \left\|\frac{u_{R,\delta}^-}{|x|}\right\| \leq \frac{2(d-1)}{d-2}\left(\Lambda\,\|\nabla u_{R,\delta}^-\|^2 + \epsilon^2(R)\,\|\nabla u_{R,\delta}^-\|\right). \tag{17.65}$$

Since $\left|\partial_r \overline{u}_{R,\delta} + i\lambda_1^{\frac{1}{2}}\,\mathrm{sgn}(\lambda_2)\,\overline{u_{R,\delta}}\right| = \left|\overline{\partial_r u_{R,\delta}^-}\right|$, we may write

$$|I_2| \leq 2\,\|x\widetilde{f}_{R,\delta}\|\|\partial_r u_{R,\delta}^-\| \leq 2\,\|x\widetilde{f}_{R,\delta}\|\|\nabla u_{R,\delta}^-\| \leq 2\left(\Lambda\,\|\nabla u_{R,\delta}^-\|^2 + \epsilon^2(R)\,\|\nabla u_{R,\delta}^-\|\right). \tag{17.66}$$

If $\lambda_2 \neq 0$, we also need to estimate the term I_3. First notice that identity (17.57) with the constant choice $G_2(x) := \frac{\lambda_2}{|\lambda_2|}$, immediately gives the L^2-bound

$$\|u_{R,\delta}\|^2 \leq |\lambda_2|^{-1} \int |\widetilde{f}_{R,\delta}||u_{R,\delta}|\,.$$

As a consequence, since $|\lambda_2| \leq \lambda_1$, we have

$$\begin{aligned}
|I_3| &\leq \frac{|\lambda_2|}{\lambda_1^{\frac{1}{2}}}\|x\widetilde{f}_{R,\delta}\|\|u_{R,\delta}\| \leq \left(\Lambda\,\|\nabla u_{R,\delta}^-\| + \epsilon^2(R)\right)\sqrt{\int |\widetilde{f}_{R,\delta}||u_{R,\delta}|} \\
&\leq \left(\Lambda\,\|\nabla u_{R,\delta}^-\| + \epsilon^2(R)\right)\|x\widetilde{f}_{R,\delta}\|^{\frac{1}{2}} \left\|\frac{u_{R,\delta}}{|x|}\right\|^{\frac{1}{2}} \\
&\leq \Lambda^{\frac{3}{2}}\frac{\sqrt{2}}{\sqrt{d-2}}\,\|\nabla u_{R,\delta}^-\|^2 + \epsilon^2(R)\frac{\sqrt{2}}{\sqrt{d-2}}\,\|\nabla u_{R,\delta}^-\|\left(\Lambda^{\frac{1}{2}}\,\|\nabla u_{R,\delta}^-\| + \epsilon(R)\right).
\end{aligned} \tag{17.67}$$

Applying the estimates (17.64), (17.65), (17.66) and (17.67) in (17.62), we obtain

$$\begin{aligned}
&\left(1 - \frac{2(2d-3)}{d-2}\Lambda - \frac{\sqrt{2}}{\sqrt{d-2}}\,\Lambda^{\frac{3}{2}}\right)\int |\nabla u_{R,\delta}^-|^2 + \frac{|\lambda_2|}{\lambda_1^{\frac{1}{2}}}\frac{d-3}{d-1}\int |x||\nabla u_{R,\delta}^-|^2 \\
&\leq \epsilon^2(R)\left\|\nabla u_{R,\delta}^-\right\|\left(\frac{4d-6}{d-2} + \frac{\sqrt{2}}{\sqrt{d-2}}\,\Lambda^{\frac{1}{2}}\|\nabla u_{R,\delta}^-\| - \frac{\sqrt{2}}{\sqrt{d-2}}\,\epsilon(R)\right).
\end{aligned}$$

For fixed R, let $\delta \to 0$ in the last inequality; since $u_{R,\delta}$ is compactly supported, by the dominated convergence theorem, one gets

$$\begin{aligned}
&\left(1 - \frac{2(2d-3)}{d-2}\Lambda - \frac{\sqrt{2}}{\sqrt{d-2}}\,\Lambda^{\frac{3}{2}}\right)\int |\nabla u_R^-|^2 + \frac{|\lambda_2|}{\lambda_1^{\frac{1}{2}}}\frac{d-3}{d-1}\int |x||\nabla u_R^-|^2 \\
&\leq \epsilon^2(R)\left\|\nabla u_R^-\right\|\left(\frac{4d-6}{d-2} + \frac{\sqrt{2}}{\sqrt{d-2}}\,\Lambda^{\frac{1}{2}}\|\nabla u_R^-\| - \frac{\sqrt{2}}{\sqrt{d-2}}\,\epsilon(R)\right).
\end{aligned}$$

Let finally $R \to \infty$; by the monotone convergence theorem and the fact that $u^- \in H^1(\mathbb{R}^d)$, we conclude that

$$\left(1 - \frac{2(2d-3)}{d-2}\Lambda - \frac{\sqrt{2}}{\sqrt{d-2}}\,\Lambda^{\frac{3}{2}}\right)\int |\nabla u^-|^2 + \frac{|\lambda_2|}{\lambda_1^{\frac{1}{2}}}\frac{d-3}{d-1}\int |x||\nabla u^-|^2 \leq 0\,. \tag{17.68}$$

By virtue of (17.50), it follows that u^- and thus u are identically equal to zero.

$\boxed{\textbf{Case } |\lambda_2| > \lambda_1.}$ Let $u \in H^1(\mathbb{R}^d)$ be a solution to (17.47). Choosing as a test function $v = \pm u$ in (17.47), and taking real and imaginary parts of the resulting identities, one easily gets

$$(\lambda_1 \pm \lambda_2) \int |u|^2 = \int |\nabla u|^2 + \Re \int f\overline{u} \pm \Im \int f\overline{u}. \tag{17.69}$$

By the Schwarz inequality, the Hardy inequality (17.6) and assumption (17.49), we estimate

$$\Re \int f\overline{u} \pm \Im \int f\overline{u} \leq 2 \int |f||u| \leq 2\, \|xf\| \left\| \frac{u}{|x|} \right\| \leq \frac{4}{d-2}\, \Lambda \int |\nabla u|^2 .$$

Consequently, (17.69) yields

$$(\lambda_1 \pm \lambda_2) \int |u|^2 \geq \left(1 - \frac{4}{d-2}\Lambda\right) \int |\nabla u|^2 .$$

Notice that (17.50) implies that $\Lambda < \frac{d-2}{4}$, therefore the last inequality forces $\lambda_1 \pm \lambda_2 \geq 0$ unless $u = 0$. Since we assume $|\lambda_2| > \lambda_1$, we conclude that $u = 0$. □

By taking $f := Vu$ in Theorem 17.8 (notice that Vu belongs to $H^{-1}(\mathbb{R}^d)$ under the hypothesis (17.70)) and using that $|u| = |u^-|$, we immediately obtain

Corollary 17.1. *Let $d \geq 3$ and suppose*

$$\forall \psi \in H^1(\mathbb{R}^d)\,, \qquad \int_{\mathbb{R}^d} |x|^2\, |V(x)|^2\, |\psi(x)|^2 \, dx \leq \Lambda^2 \int_{\mathbb{R}^d} |\nabla \psi|^2 \,, \tag{17.70}$$

where Λ satisfies (17.50). *Then $\sigma_{\mathrm{p}}(H_V) = \varnothing$.*

Proof. In fact, Theorem 17.8 only gives the weaker conclusion that no complex point λ satisfying $\Re\lambda > 0$ can be an eigenvalue of H_V. However, (17.70) with (17.50) implies (17.1), which in turn yields that all possible eigenvalues of H_V are included in the right complex plane, *i.e.* $\Re\lambda > 0$. Indeed, this fact follows from the identity

$$\int |\nabla u|^2 + \Re \int V|u|^2 = \Re\lambda \int |u|^2 \,, \tag{17.71}$$

which can be obtained from (17.56) with the constant choice $G_1 := 1$ and $f := Vu$. □

Now we are in a position to prove Theorem 17.2.

Proof of Theorem 17.2. Theorem 17.2 follows as a weaker version of Corollary 17.1. Indeed, it is easy to see that any Λ verifying (17.50) necessarily satisfies $\Lambda \leq (d-2)/2$. Using the latter in the former, we obtain (17.10) as a sufficient condition which guarantees (17.70). □

We now turn our attention to Theorem 17.3. In analogy with the above strategy, we first study the (more difficult) part $\Re\lambda > 0$. In the following, we set $V_1 := \Re V$ and $V_2 := \Im V$.

Theorem 17.9. *Let $d \geq 3$. Let $u \in \mathcal{D}(\mathbb{R}^d)$ be a solution of* (17.46) *with $\Re\lambda > 0$, and let $f := Vu$ where V satisfies* (17.14), (17.15), (17.16) *and* (17.13). *Then $u = 0$.*

Proof. The proof is completely analogous to that of Theorem 17.8. The only difference consists in the way we handle the right-hand side of (17.62), as we see in the sequel.

$\boxed{\textbf{Case } |\lambda_2| \leq \lambda_1.}$ With the same notations as above, if $u \in \mathcal{D}(\mathbb{R}^d) \subset H^1(\mathbb{R}^d)$ solves (17.46), then identity (17.62) holds. We now need to rewrite the right-hand side of (17.62) in a suitable way. To this aim, recall that $\widetilde{f}_R$ is defined via (17.52), where $f := Vu$. It is convenient to introduce the notation

$$K_R(u, \nabla u) := -2\nabla\xi_R \cdot \nabla u - u\Delta\xi_R. \tag{17.72}$$

so that $\widetilde{f}_R = f_R + K_R(u,\nabla u)$. Putting (17.72) into (17.62), integrating by parts in the first two terms involving V_1 and taking the limit as $\delta \to 0$, one gets the following key identity:

$$\begin{aligned} I := \int \left|\nabla u_R^-\right|^2 + \frac{|\lambda_2|}{\lambda_1^{\frac12}} \int |x||\nabla u_R^-|^2 - \frac{(d-1)}{2}\frac{|\lambda_2|}{\lambda_1^{\frac12}} \int \frac{|u_R|^2}{|x|} - \frac{|\lambda_2|}{\lambda_1^{\frac12}} \int |x| V_1 |u_R|^2 \\ = \underbrace{\int |u_R^-|^2 \left(V_1 + |x|\partial_r V_1\right)}_{I_1} + \underbrace{2\Im \int |x| V_2 u_R \left(\partial_r \overline{u_R} + i\,\mathrm{sgn}(\lambda_2)\lambda_1^{\frac12}\overline{u_R}\right)}_{I_2} \\ \underbrace{+ (1-d)\Re \int K_R(u,\nabla u)\overline{u_R} - 2\Re \int |x| K_R(u,\nabla u)\left(\partial_r\overline{u_R} + i\,\mathrm{sgn}(\lambda_2)\lambda_1^{\frac12}\overline{u_R}\right) - \frac{\lambda_2}{\lambda_1^{\frac12}}\Re \int |x| K_R(u,\nabla u)\overline{u_R}}_{I_3}\,. \end{aligned} \tag{17.73}$$

We start by estimating the individual terms on the right hand side of (17.73). Thanks to assumption (17.15), we have

$$I_1 = \int |u_R^-|^2 \partial_r(|x|V_1) \le \int |u_R^-|^2 \left[\partial_r(|x|V_1)\right]_+ \le b_2^2 \int |\nabla u_R^-|^2. \tag{17.74}$$

We now use $\left|\partial_r \overline{u}_R + i\lambda_1^{\frac12}\,\mathrm{sgn}(\lambda_2)\,\overline{u_R}\right| = \left|\overline{\partial_r u_R^-}\right|$ to write

$$|I_2| \le 2\|xV_2 u_R\|\|\partial_r u_R^-\| \le 2\|xV_2 u_R\|\|\nabla u_R^-\| \le 2b_3 \int |\nabla u_R^-|^2. \tag{17.75}$$

Finally, by (17.51) and the fact that $u_R \in H^1(\mathbb{R}^d)$, one easily gets that

$$|I_3| \le \epsilon^2(R), \qquad \lim_{R\to\infty} \epsilon^2(R) = 0. \tag{17.76}$$

We now proceed by estimating the left-hand side of (17.73) from below. By (17.14) we obtain

$$\frac{|\lambda_2|}{\lambda_1^{\frac12}} \int |x| V_1 |u_R|^2 \ge -\frac{|\lambda_2|}{\lambda_1^{\frac12}} \int (V_1)_- \left||x|^{\frac12} u_R^-\right|^2 \ge -b_1^2 \frac{|\lambda_2|}{\lambda_1^{\frac12}} \int \left|\nabla\left(|x|^{\frac12} u_R^-\right)\right|^2. \tag{17.77}$$

Now write

$$\frac{|\lambda_2|}{\lambda_1^{\frac12}} \int |x||\nabla u_R^-|^2 - \frac{(d-1)}{2}\frac{|\lambda_2|}{\lambda_1^{\frac12}} \int \frac{|u_R|^2}{|x|} = \frac{|\lambda_2|}{\lambda_1^{\frac12}} \int \left|\nabla\left(|x|^{\frac12} u_R^-\right)\right|^2 - \frac14 \frac{|\lambda_2|}{\lambda_1^{\frac12}} \int \frac{\left|u_R^-\right|^2}{|x|}. \tag{17.78}$$

Notice that identity (17.57) with the constant choice $G_2(x) := \frac{\lambda_2}{|\lambda_2|}$, in the limit as $\delta \to 0$, reads as follows

$$|\lambda_2| \int |u_R|^2 = \frac{\lambda_2}{|\lambda_2|} \int V_2 |u_R|^2 + \frac{\lambda_2}{|\lambda_2|} \Im \int K_R(u,\nabla u)\overline{u_R}.$$

Since $u_R \in H^1(\mathbb{R}^d)$, arguing as in (17.11), by (17.16), (17.51) and the fact that $|u_R| = |u_R^-|$, we obtain the L^2-bound

$$\|u_R\|^2 \le |\lambda_2|^{-1} \left(\frac{2b_3}{d-2} \int |\nabla u_R^-|^2 + \epsilon^2(R)\right), \qquad \lim_{R\to\infty} \epsilon^2(R) = 0. \tag{17.79}$$

As a consequence of (17.79), since $|\lambda_2| \le \lambda_1$, we can estimate the last term in (17.78), by the Schwarz and Hardy inequalities as follows:

$$\frac{|\lambda_2|}{\lambda_1^{\frac12}} \int \frac{\left|u_R^-\right|^2}{|x|} \le \frac{|\lambda_2|}{\lambda_1^{\frac12}} \left\|\frac{u_R^-}{|x|}\right\| \|u_R^-\| \le \sqrt{b_3}\left(\frac{2}{d-2}\right)^{\frac32} \int \left|\nabla u_R^-\right|^2 + \frac{2}{d-2}\|\nabla u_R^-\|\,|\epsilon(R)|, \tag{17.80}$$

where $\epsilon(R)$ is the error term from (17.79). By (17.77), (17.78), and (17.80), we conclude that

$$I \ge \left[1 - \frac14\sqrt{b_3}\left(\frac{2}{d-2}\right)^{\frac32}\right] \int \left|\nabla u_R^-\right|^2 - \frac14 \frac{2}{d-2}\|\nabla u_R^-\|\,|\epsilon(R)|. \tag{17.81}$$

Applying (17.74), (17.75), (17.76) and (17.81) in (17.73), we obtain

$$\left[1 - b_2^2 - 2\,b_3 - \frac14\sqrt{b_3}\left(\frac{2}{d-2}\right)^{\frac32}\right] \int \left|\nabla u_R^-\right|^2 \le \epsilon^2(R) + \frac14\frac{2}{d-2}\|\nabla u_R^-\|\,|\epsilon(R)|,$$

for any $R > 0$, with $\lim_{R\to\infty} \epsilon^2(R) = 0$. In the limit as $R \to \infty$, by the monotone convergence theorem, we finally get

$$\left[1 - b_2^2 - 2\,b_3 - \frac{1}{4}\sqrt{b_3}\left(\frac{2}{d-2}\right)^{\frac{3}{2}}\right] \int \left|\nabla u^-\right|^2 \le 0\,. \tag{17.82}$$

By virtue of (17.13), it follows that u^- and thus u are identically equal to zero.

$\boxed{\textbf{Case } |\lambda_2| > \lambda_1\textbf{.}}$ The proofs in this case is based on identity (17.69). When $f := Vu$, it reads as follows:

$$(\lambda_1 \pm \lambda_2)\int |u|^2 = \int |\nabla u|^2 + \int V_1|u|^2 \pm \int V_2|u|^2 \ge \int |\nabla u|^2 - \int (V_1)_-|u|^2 - \left|\int V_2|u|^2\right|. \tag{17.83}$$

By means of (17.11), (17.14) and (17.16), we have

$$(\lambda_1 \pm \lambda_2)\int |u|^2 \ge \left[1 - b_1^2 - \frac{2b_3}{d-2}\right]\int |\nabla u|^2.$$

Therefore, condition (17.13) implies that $\lambda_1 \pm \lambda_2 \ge 0$, and since $|\lambda_2| > \lambda_1$ we conclude that u is identically zero. ☐

Now we are in a position to prove Theorem 17.3.

Proof of Theorem 17.3. Theorem 17.9 implies that $\sigma_{\mathrm{p}}(H_V) \cap \{\lambda_1 > 0\} = \varnothing$. In addition, if $\lambda_1 \le 0$, then choosing $v := u$ in (17.47) and taking the resulting real part, one obtains

$$\lambda_1 \int |u|^2 = \int |\nabla u|^2 + \int V_1\,|u|^2 \ge \int |\nabla u|^2 - \int (V_1)_-\,|u|^2 \ge (1 - b_1^2)\int |\nabla u|^2\,,$$

where the last inequality follows by (17.14). This implies that $\sigma_{\mathrm{p}}(H_V) \cap \{\lambda_1 \le 0\} = \varnothing$, so the proof is completed. ☐

We conclude the manuscript with the proof of Theorem 17.4. Since the strategy is identical to the proof of Theorem 17.3, we just sketch it.

Proof of Theorem 17.4. Equation (17.46) is now replaced by

$$\Delta_A u + \lambda u = Vu\,, \tag{17.84}$$

where $\Delta_A := \nabla_A \cdot \nabla_A$. Let $u \in \mathcal{D}_A(\mathbb{R}^d)$ be a weak solution to (17.84). By similar algebraic manipulations as in the proof of Theorem 17.3, we get an analogue to (17.73):

$$\begin{aligned}
&\int \left|\nabla_A u_R^-\right|^2 + \frac{|\lambda_2|}{\lambda_1^{\frac{1}{2}}}\frac{d-3}{d-1}\int |x||\nabla_A u_R^-|^2 \le \int |u_R|^2\,(V_1 + |x|\partial_r V_1) - \frac{|\lambda_2|}{\lambda_1^{\frac{1}{2}}}\int |x|V_1|u_R|^2 \\
&+ 2\Im\int |x|u_R V_2\left(\overline{\partial_r^A u_R} + i\,\mathrm{sgn}(\lambda_2)\lambda_1^{\frac{1}{2}}\overline{u_R}\right) + 2\Im\int |x|u_R B_\tau\cdot\overline{\nabla_A u_R} \\
&+ (1-d)\Re\int K_R(u,\nabla_A u)\overline{u_R} - 2\Re\int |x|K_R(u,\nabla_A u)\left(\partial_r^A\overline{u_R} + i\,\mathrm{sgn}(\lambda_2)\lambda_1^{\frac{1}{2}}\overline{u_R}\right) \\
&- \frac{\lambda_2}{\lambda_1^{\frac{1}{2}}}\Re\int |x|K_R(u,\nabla_A u)\overline{u_R}\,,
\end{aligned}$$

where $\partial_r^A := \frac{x}{|x|}\cdot\nabla_A$. In fact, in order to obtain the last identity, one proceeds exactly as above, with the only difference arising once obtaining identity (17.58), in which we use the test function $v := \nabla G_3\cdot\nabla_A u_{R,\delta} + \Delta G_3 u_{R,\delta}$. The key remark is that B_τ is a tangential vector, so that

$$|B_\tau\cdot\nabla_A u_R| = \left|B_\tau\cdot\left(\nabla_A u_R + i\,\mathrm{sgn}(\lambda_2)\lambda_1^{\frac{1}{2}}\frac{x}{|x|}u_R\right)\right| = \left|B_\tau\cdot\nabla_A u_R^-\right|\,,$$

and we can rewrite the last inequality as

$$\begin{aligned}
&\int \left|\nabla_A u_R^-\right|^2 + \frac{|\lambda_2|}{\lambda_1^{\frac{1}{2}}}\frac{d-3}{d-1}\int |x||\nabla_A u_R^-|^2 \\
&\leq \int |u_R|^2\,(V_1 + |x|\partial_r V_1) - \frac{|\lambda_2|}{\lambda_1^{\frac{1}{2}}}\int |x|V_1|u_R|^2 + 2\Im\int |x|u_R\overline{\nabla_A u_R}\cdot\left(V_2\frac{x}{|x|} + B_\tau\right) \\
&\quad + (1-d)\Re\int K_R(u,\nabla_A u)\overline{u_R} - 2\Re\int |x|K_R(u,\nabla_A u)\left(\partial_r^A\overline{u_R} + i\,\mathrm{sgn}(\lambda_2)\lambda_1^{\frac{1}{2}}\overline{u_R}\right) \\
&\quad - \frac{\lambda_2}{\lambda_1^{\frac{1}{2}}}\Re\int |x|K_R(u,\nabla_A u)\overline{u_R}\,.
\end{aligned}$$

One now proceeds in the same way as in the magnetic-free case, to conclude that $u = 0$ if $\Re\lambda > 0$. To complete the proof, we then argue exactly as above; we omit further details. □

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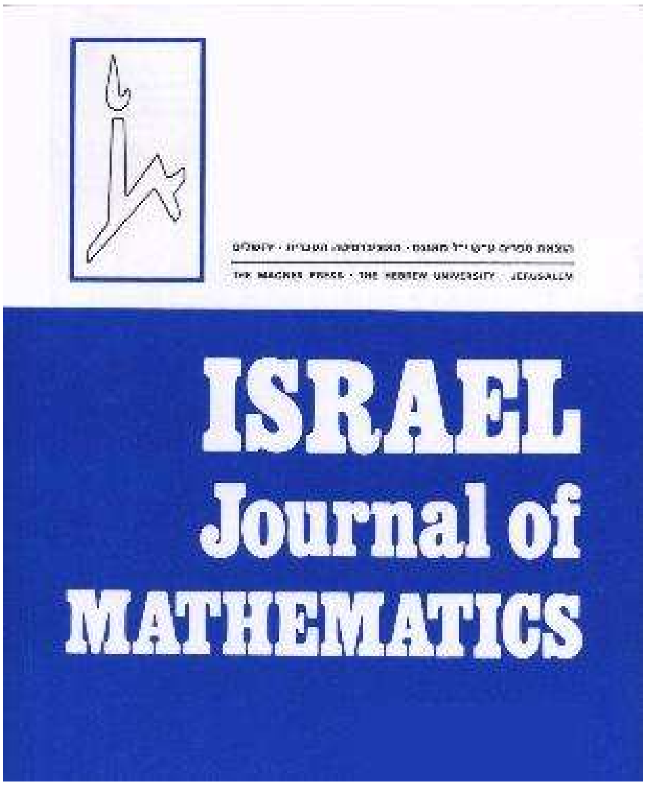
Chapter 18

Non-accretive Schrödinger operators and exponential decay of their eigenfunctions



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Non-accretive Schrödinger operators and exponential decay of their eigenfunctions

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Abstract. We consider non-self-adjoint electromagnetic Schrödinger operators on arbitrary open sets with complex scalar potentials whose real part is not necessarily bounded from below. Under a suitable sufficient condition on the electromagnetic potential, we introduce a Dirichlet realisation as a closed densely defined operator with non-empty resolvent set and show that the eigenfunctions corresponding to discrete eigenvalues satisfy an Agmon-type exponential decay.

Keywords: Schrödinger operators, complex potentials, Agmon estimates, domain separation

18.1 Introduction

18.1.1 Context and motivation

We consider the electromagnetic Schrödinger operator

$$(-i\nabla + \mathbf{A})^2 + V \qquad \text{in} \qquad L^2(\Omega)\,, \tag{18.1}$$

subject to Dirichlet boundary conditions on $\partial\Omega$, where Ω is an arbitrary open subset of $\mathbb{R}^d$. The functions $V : \Omega \to \mathbb{C}$ and $\mathbf{A} : \Omega \to \mathbb{R}^d$ are the scalar (electric) and vector (magnetic) potentials, respectively.

If $d = 3$ and V is real-valued, the self-adjoint Dirichlet realisation of (18.1) is the Hamiltonian of a quantum particle constrained to a nanostructure Ω and subjected to an external electromagnetic field $(-\operatorname{grad} V, -\operatorname{rot}\mathbf{A})$. The literature on the subject is enormous and we restrict ourselves to referring to the recent book [24] with an extensive bibliography.

Although complex-valued potentials V have appeared in quantum theory from its early years, too, notably in the context of effective Hamiltonians for open systems (see, e.g., [16]) and resonances (see [1] for a more recent study), the corresponding spectral theory is much less developed. The interest in non-self-adjoint Schrödinger operators have been renewed at the turn of the millenium with the advent of the so-called quasi-Hermitian quantum mechanics (see [22] for a mathematically oriented review). There are also motivations in other areas of physics, for instance, superconductivity (see [3] for a mathematical treatement) and optics with a number of recent experiments (see, e.g., [25]). Finally, Schrödinger operators with potentials having a complex coupling constant (in fact spectral parameter) appear naturally in the study of the damped wave equation (see, e.g., [28, 7]).

18.1.2 About the main results

Our main result is the Agmon-type exponential decay of eigenfunctions corresponding to discrete eigenvalues of (18.1), cf. Theorem 18.4, which can be viewed as a non self-adjoint version of the Agmon-Persson estimates, see [23, 2]. We emphasise that the decay is *not* an effect of the positive part of $\Re V$ since it may be absent, or even worse, $\Re V$ is allowed to be negative and unbounded at infinity.

A sufficient condition to define the operator

The first problem that we tackle in our analysis is finding of a Dirichlet realisation of (18.1) with *non-empty resolvent set*. This is not a trivial task as we do not restrict the signs of $\Re V$ and $\Im V$ and so the standard sectorial form techniques of [16, Sec. VI.2.1] are not available.

A simple example one should have in mind is

$$-\frac{\mathrm{d}^2}{\mathrm{d}x^2} - x^2 + ix^3 \qquad \text{in} \qquad L^2(\mathbb{R})\,, \tag{18.2}$$

for which the numerical range covers the whole complex plane. Due to the latter, even the Kato's theorem for accretive Schrödinger operators, based on Kato's distributional inequality [8, Sec. VII.2], is not applicable immediately.[1] Here we can even go beyond operators like (18.2) for which the suitable Dirichlet realisation can be actually found by available methods in [4, 5]. We allow much wilder behaviour of V in terms of the possible growth at infinity and oscillations. In more detail, we essentially require that (cf. Assumption 18.1 and Proposition 18.1)

$$|\nabla V(x)| + |\nabla \mathbf{B}(x)| = o\left((|V(x)| + |\mathbf{B}(x)|)^{\frac{3}{2}} + 1\right), \tag{18.3}$$

$$(\Re V(x))_- = o\Big(|V(x)| + |\mathbf{B}(x)| + 1\Big), \tag{18.4}$$

as $|x| \to \infty$, where $(\Re V)_-$ is the negative part of $\Re V$ and $\mathbf{B} := \mathrm{d}\mathbf{A}$ is the magnetic matrix.

The condition (18.4) puts restrictions on the size of $(\Re V)_-$ which in fact represents a "small" perturbation of an m-accretive operator (18.1) with V replaced by $(\Re V)_+ + i\,\Im V$. Notice however, that $(\Re V)_-$ can be compensated not only by $\Im V$, but also by the magnetic field. In a different context (absence of eigenvalues), a certain analogy between the magnetic field and $\Im V$ was observed in [17].

About the power $\frac{3}{2}$

The power $\frac{3}{2}$ in the condition (18.3) is an improvement comparing to [4, 5] where the power 1 is assumed; in these references (where (18.2) fits already), a big-$\mathcal{O}$ instead of the little-o is used. In the present paper, we can therefore treat examples like

$$-\frac{\mathrm{d}^2}{\mathrm{d}x^2} - e^{x^2} + ie^{x^4} \qquad \text{in} \qquad L^2(\mathbb{R})\,. \tag{18.5}$$

Moreover, we show in Theorem 18.2 that the operator domain of the found realisation of (18.1) possesses a very convenient separation property, namely

$$\mathsf{D}((-i\nabla + \mathbf{A})^2 + V) = \mathsf{D}((-i\nabla + \mathbf{A})^2) \cap \mathsf{D}(V)\,. \tag{18.6}$$

The power $\frac{3}{2}$ in (18.3) is not a coincidence as it is known to be optimal (with little-o replaced by a sufficiently small constant in (18.3)) with respect to the separation property in the self-adjoint case [14, 15, 8] (see also [11], [20] in the magnetic case).

Weighted coercivity

Our approach for proving all the results of this paper is based on the generalised Lax-Milgram-type theorem of Almog and Helffer [4] involving a new idea of *weighted coercivity*, which can be viewed as a generalisation of the $\mathbb{T}$-coercivity (see for instance [6, Def. 2.1]). While from the point of view of abstract Lax-Milgram or representation theorems, an optimal "if and only if" condition for m-accretivity was found in the recent work [29, Thm. 4.2], the weighted coercivity of Theorem 18.7 makes such abstract results directly applicable for (18.1). Moreover, the present paper reveals a connection between weighted coercivity and exponential decay of eigenfunctions stated in Theorem 18.4.

18.1.3 Examples of applications

Besides the independent interest of our results, we indicate below two connections to other recent works, both when $|V|$ is confining so that the resolvent of (18.1) is compact (see Proposition 18.2). The first one concerns the completeness of eigensystem of (18.1), the second one the rates of eigenvalue convergence of domain truncations.

Eigensystem completeness

The crucial ingredient in a natural proof of the eigensystem completeness is the fundamental result of operator theory (see, e.g., [12, Cor. XI.9.31]) combining the p-Schatten class property of the resolvent and a control of the resolvent norm on a sufficient number of rays in $\mathbb{C}$; for operators like (18.1), this approach was followed in [27, 4]. We indicate how the completeness results can be extended to operators satisfying weaker conditions (18.3) only. Our domain separation and the graph norm estimate (cf. Theorem 18.2), the second resolvent identity and the ideal property of Schatten classes show that the resolvent of (18.1) is in the p-Schatten class ($0 < p < \infty$) if and only if the resolvent of the self-adjoint (18.1) with V replaced by $|V|$ is in the p-Schatten class; to obtain

[1] Note that, in special self-adjoint settings, however, interesting alternative approaches can be found in the literature. For instance, in [19], representation theorems for indefinite quadratic forms are established and can be used to define certain self-adjoint operators possibly unbounded from below.

the value of p depending on V and $\mathbf{A}$, criteria of the type [4, Thm. 1.3] can be applied. To have the control of the resolvent norm on rays in $\mathbb{C}$, we can use the standard bound (1 over the distance to the numerical range) if (18.1) is at least accretive and, in the non-accretive case, the perturbation result [16, Thm. IV.3.17] with viewing $(\Re V)_-$ as a relatively bounded perturbation of an m-accretive operator (18.1) with V replaced by $(\Re V)_+ + i\,\Im V$ (see [5, Prop. 2.4 (iv)] for details on such an approach).

Domain truncation

It was proved in [5] that eigenvalues of (18.1) on $\mathbb{R}^d$ with $\mathbf{A} = 0$ and V satisfying (stronger) conditions of the type (18.3)–(18.4), see [5, Asm. II], can be approximated without pollution by the eigenvalues of (18.1) truncated to a sequence of expanding domains, e.g. balls, and subject to Dirichlet boundary conditions. The rate of convergence for a given eigenvalue of (18.1) on $\mathbb{R}^d$ was estimated by the decay rate of the corresponding eigenfunctions (and generalised eigenfunctions in the case of Jordan blocks) at infinity (see [5, Thm. 5.2]). Our Agmon-type estimate (cf. Theorem 18.4 and Remark 18.3) shows that this convergence is exponential which vastly generalises known facts for complex polynomial potentials (see, e.g., [26, 9]).

18.1.4 Organisation of the paper

In Section 18.2, we summarise our main results. The definition of (18.1) as a closed densely defined operator together with a convenient characterisation of the operator domain is performed in Section 18.3. The spectral properties are established in Section 18.4. At the end of the paper, we attach Appendix 18.5 with elements of spectral theory related to the present study.

18.2 Main results

18.2.1 Assumptions

Let Ω be a non-empty open (possibly unbounded) subset of $\mathbb{R}^d$, $d \geq 1$. Another standing assumption of this paper is that the electromagnetic potentials satisfy

$$(V, \mathbf{A}) \in \mathcal{C}^1(\bar{\Omega}; \mathbb{C}) \times \mathcal{C}^2(\bar{\Omega}; \mathbb{R}^d)\,.$$

This smoothness hypothesis is technically convenient, but it is definitely far from being optimal for the applicability of our techniques and the validity of the obtained results. We write $V = V_1 + iV_2$ where V_1 and V_2 are real-valued. Associated with the vector potential $\mathbf{A}$, we consider the magnetic (skew-symmetric) matrix

$$\mathbf{B} = (B_{jk})_{j,k\in\{1,\dots,d\}}\,, \qquad B_{jk} := \partial_j A_k - \partial_k A_j = i[P_j, P_k]\,, \tag{18.7}$$

where $P_\ell := -i\partial_\ell + A_\ell$.

As in [4], let us introduce functions

$$\Phi := \frac{V_2}{m_{\mathbf{B},V}} \qquad \text{and} \qquad \Psi := \frac{\mathbf{B}}{m_{\mathbf{B},V}}\,, \tag{18.8}$$

where

$$m_{\mathbf{B},V} := \sqrt{1 + |\mathbf{B}|^2 + |V|^2}\,.$$

Here $|V(x)|$ denotes the usual norm of a complex number, while we use

$$|\mathbf{B}(x)| := \sqrt{\sum_{j,k=1}^{d} B_{jk}(x)^2}\,, \qquad |\nabla\mathbf{B}(x)| := \sqrt{\sum_{j,k=1}^{d} |\nabla B_{jk}(x)|^2}\,,$$

where $|\nabla B_{jk}(x)|$ is now the usual Euclidean norm of a vector in $\mathbb{R}^d$. Finally, given a real-valued function a, we adopt the standard notation $a_\pm := \max(\pm a, 0)$.

With these notations, the main hypothesis of this paper reads:

Assumption 18.1. There exist constants $\gamma_1 > 0$ and $\gamma_2 \in \mathbb{R}$ such that

$$\frac{V_2^2 + \frac{1}{12d}|\mathbf{B}|^2}{m_{\mathbf{B},V}} + V_1 - 9\left(|\nabla\Phi|^2 + |\nabla\Psi|^2\right) \geq \gamma_1 m_{\mathbf{B},V} - \gamma_2\,. \tag{18.9}$$

Remark 18.1. On the left-hand side in (18.9), the first term is non-negative, the last bracket gives a non-positive contribution and V_1 has no sign *a priori*. If V_1 is bounded from below, then we only have to control the last term to obtain the required inequality. The point is that V_2 or $\mathbf{B}$ can be used to control the non-positive contribution of V_1. Note also that we can replace the assumption (18.9) by the weaker one:

$$\frac{V_2^2 + \frac{1}{12d}|\mathbf{B}|^2}{m_{\mathbf{B},V}} + V_1 - 9\left(|\nabla\Phi|^2 + |\nabla\Psi|^2\right) \geq \gamma_1|V| - \gamma_2\,, \tag{18.10}$$

up to slight modifications of our variational framework.

Assumption 18.1 is easily checked to hold for (18.2). A sufficient condition for the validity of Assumption 18.1 is contained in the following proposition.

Proposition 18.1. *Suppose*

$$|\nabla V(x)| + |\nabla \mathbf{B}(x)| = o\left(m_{\mathbf{B},V}^{\frac{3}{2}}(x)\right), \tag{18.11}$$

$$\left(V_1\right)_-(x) = o\left(m_{\mathbf{B},V}(x)\right), \tag{18.12}$$

as $|x| \to +\infty$. *Then Assumption 18.1 is satisfied.*

18.2.2 Definition of the operator

First we introduce the usual magnetic Sobolev space

$$H^1_{\mathbf{A}}(\Omega) := \{u \in L^2(\Omega) \,:\, (-i\nabla + \mathbf{A})u \in L^2(\Omega)\}\,,$$

equipped with the norm

$$\|u\|_{H^1_{\mathbf{A}}(\Omega)} := \sqrt{\|u\|^2 + \|(-i\nabla + \mathbf{A})u\|^2}\,.$$

Here $\|\cdot\|$ denotes the norm of $L^2(\Omega)$ and the associated inner product will be denoted by $\langle\cdot,\cdot\rangle$. We also introduce the subspace $H^1_{\mathbf{A},0}(\Omega)$ defined as the closure of $\mathcal{C}_0^\infty(\Omega)$ for the norm $\|\cdot\|_{H^1_{\mathbf{A}}(\Omega)}$. Then we can introduce our variational space as

$$\mathscr{V} := \left\{u \in H^1_{\mathbf{A},0}(\Omega) \,:\, m_{\mathbf{B},V}^{\frac{1}{2}} u \in L^2(\Omega)\right\}\,,$$

equipped with the norm

$$\|u\|_{\mathscr{V}} := \sqrt{\|u\|^2_{H^1_{\mathbf{A}}(\Omega)} + \int_\Omega m_{\mathbf{B},V}|u|^2\,\mathrm{d}x}\,,$$

with respect to which $\mathscr{V}$ is complete.

We introduce a sesquilinear form

$$Q(u,v) := \langle(-i\nabla + \mathbf{A})u, (-i\nabla + \mathbf{A})v\rangle + \int_\Omega V u\bar{v}\,\mathrm{d}x\,, \qquad \mathsf{D}(Q) := \mathscr{V}\,.$$

For $u, v \in \mathcal{C}_0^\infty(\Omega)$, a dense subspace of $\mathscr{V}$, we have

$$Q(u,v) = \left\langle(-i\nabla + \mathbf{A})^2 u + Vu, v\right\rangle\,,$$

so Q is the form naturally associated with (18.1). If V were such that Q was sectorial, then Q would be closed and it would give rise to an m-sectorial operator by Kato's representation theorem [21, Thm. VI.2.1]. In our general setting (where the numerical range of Q is allowed to be the whole complex plane), however, there is no general representation theorem and even the notion of closedness for forms is not standard. Anyway, we are still allowed to introduce *an* operator $\mathscr{L}$ by the Riesz theorem

$$\forall u \in \mathsf{Dom}(\mathscr{L}), \quad \forall v \in \mathscr{V}, \qquad Q(u,v) =: \langle\mathscr{L}u, v\rangle\,, \tag{18.13}$$

where

$$\mathsf{Dom}(\mathscr{L}) := \big\{v \in \mathscr{V} \,: \quad u \mapsto Q(u,v) \text{ is continuous on } \mathscr{V} \text{ for the norm of } L^2(\Omega)\big\}\,. \tag{18.14}$$

The following theorem shows that such a defined operator $\mathscr{L}$ shares all the nice properties of operators introduced by the standard representation theorem. The proof is based on the new abstract representation theorem of Almog and Helffer (see [4, Thm. 2.2], reproduced below as Theorem 18.6).

Theorem 18.1. *Suppose Assumption 18.1. The following properties hold:*

(i) $\mathsf{Dom}(\mathscr{L})$ *is dense in* $L^2(\Omega)$,

(ii) $\mathscr{L}$ *is closed,*

(iii) *the resolvent set of* $\mathscr{L}$ *is not empty.*

Furthermore, we have the following description of the domain of $\mathscr{L}$.

Theorem 18.2. *Let* (18.11) *and* (18.12) *hold. Then we have*

$$\mathsf{Dom}(\mathscr{L}) = \left\{u \in \mathscr{V} \,:\, (-i\nabla + \mathbf{A})^2 u \in L^2(\Omega) \ \wedge\ Vu \in L^2(\Omega)\right\} .$$

Moreover, for every $\delta > 0$*, there exists* $C_\delta > 0$ *such that, for all* $u \in \mathsf{Dom}(\mathscr{L})$,

$$\|\mathscr{L}u\|^2 \geq (1-\delta)\left(\|(-i\nabla + \mathbf{A})^2 u\|^2 + \|Vu\|^2\right) - C_\delta \|u\|^2. \tag{18.15}$$

18.2.3 Spectral properties

The reader may wish to consult Appendix 18.5, where we recall basic definitions related to the spectrum and Fredholm properties.

First of all, we give a sufficient condition for $\mathscr{L}$ to have a purely discrete spectrum.

Proposition 18.2. *Suppose Assumption 18.1. If*

$$\lim_{|x|\to+\infty} m_{\mathbf{B},V}(x) = +\infty\,, \tag{18.16}$$

then $\mathscr{L}$ *is an operator with compact resolvent.*

In general, we give an estimate on the location of the essential spectrum. To this purpose, let us introduce the quantity (which is either a finite non-negative number or infinity)

$$m_\infty := \liminf_{|x|\to+\infty} m_{\mathbf{B},V}(x)\,,$$

and the following family of subsets of the complex plane:

$$\rho_c := \{\mu \in \mathbb{C} \,:\, -c - \Re\mu - |\Im\mu| > 0\}\ ,$$

where c is any real number.

Theorem 18.3. *Suppose Assumption 18.1. We have*

$$\rho_{\gamma_2} \subset \rho(\mathscr{L})\,. \tag{18.17}$$

Moreover, assuming that m_∞ *is positive, we have*

$$\rho_{\gamma_2} \subset \rho_{\gamma_2 - \gamma_1 \check{m}_\infty} \subset \mathsf{Fred}_0(\mathscr{L}) \tag{18.18}$$

for all $\check{m}_\infty \in (0, m_\infty)$*. The spectrum of* $\mathscr{L}$ *contained in* $\rho_{\gamma_2-\gamma_1\check{m}_\infty}$*, if it exists, is formed by isolated eigenvalues with finite algebraic multiplicity.*

Remark 18.2. When $m_\infty = +\infty$, we recover from Theorem 18.3 the result of Proposition 18.2.

Finally, we state our main result. It shows in particular that the discrete spectrum in the region $\rho_{\gamma_2-\gamma_1\check{m}_\infty}$ is associated with exponentially decaying eigenfunctions and that this decay may be estimated in terms of an Agmon-type distance.

Theorem 18.4. *Suppose Assumption 18.1. Let us assume that*

$$\mathsf{sp}(\mathscr{L}) \cap \rho_{\gamma_2-\gamma_1\check{m}_\infty} \neq \emptyset$$

and consider λ *in this set. Let us define the metric*

$$g(x) := \left(\gamma_1 m_{\mathbf{B},V}(x) - \Re(\lambda) - |\Im(\lambda)| - \gamma_2\right)_+ \,\mathrm{d}x^2\,,$$

and the corresponding Agmon distance *(to any fixed point of* Ω*)* $\mathrm{d}_{\mathsf{Ag}}(x)$ *that satisfies*

$$|\nabla \mathrm{d}_{\mathsf{Ag}}|^2 = \left(\gamma_1 m_{\mathbf{B},V} - \Re(\lambda) - |\Im(\lambda)| - \gamma_2\right)_+ \,. \tag{18.19}$$

Pick up any $\varepsilon \in (0,1)$*. If* ψ *is an eigenfunction associated with* λ*, we have*

$$e^{\frac{1-\varepsilon}{3}\mathrm{d}_{\mathsf{Ag}}}\,\psi \in L^2(\Omega)\,. \tag{18.20}$$

The same conclusion holds for all ψ *in the algebraic eigenspace associated with* λ.

Remark 18.3. If there exist $R > 0$ and $\gamma > 0$ such that,

$$\forall |x| \geq R\,, \qquad \gamma_1 m_{\mathbf{B},V} - \Re(\lambda) - |\Im(\lambda)| - \gamma_2 \geq \gamma\,,$$

then there exists $M \geq 0$ such that, in this region, $\mathrm{d}_{\mathsf{Ag}}(x) \geq \gamma\,|x| - M$.

Remark 18.4. In relation to Remark 18.1, if one replaced (18.9) by (18.10), the metric $g(x)$ would be changed into

$$(\gamma_1 |V(x)| - \Re(\lambda) - |\Im(\lambda)| - \gamma_2)_+ \, \mathrm{d}x^2\,,$$

and thus the weaker assumption would lead to a weaker decay of eigenfunctions.

18.3 Weighted coercivity and representation theorems

The main objective of this section is to prove Theorems 18.1 and 18.2.

18.3.1 Two abstract representation theorems

We first recall the following generalised representation theorems from [4].

Theorem 18.5 ([4, Thm. 2.1])**.** *Let $\mathcal{V}$ be a Hilbert space. Let Q be a continuous sesquilinear form on $\mathcal{V} \times \mathcal{V}$. Assume that there exist $\Phi_1, \Phi_2 \in \mathcal{L}(\mathcal{V})$ and $\alpha > 0$ such that for all $u \in \mathcal{V}$ we have*

$$|Q(u,u)| + |Q(\Phi_1(u), u)| \geq \alpha\, \|u\|_{\mathcal{V}}^2\,,$$
$$|Q(u,u)| + |Q(u, \Phi_2(u))| \geq \alpha\, \|u\|_{\mathcal{V}}^2\,.$$

The operator $\mathscr{A}$ defined by

$$\forall u, v \in \mathcal{V}, \quad Q(u,v) = \langle \mathscr{A} u, v\rangle_{\mathcal{V}}$$

is a continuous isomorphism of $\mathcal{V}$ onto $\mathcal{V}$ with bounded inverse.

Theorem 18.6 ([4, Thm. 2.2])**.** *In addition to the hypotheses of Theorem 18.5, assume that H is a Hilbert space such that $\mathcal{V}$ is continuously embedded and dense in H and that Φ_1 and Φ_2 extend to bounded operators on H. Then the operator $\mathscr{L}$ defined by*

$$\forall u \in \mathsf{Dom}(\mathscr{L}), \quad \forall v \in \mathcal{V}, \qquad Q(u,v) =: \langle \mathscr{L} u, v\rangle_{\mathsf{H}}$$

where

$$\mathsf{Dom}(\mathscr{L}) := \big\{u \in \mathcal{V} : \\ \text{the map } v \mapsto Q(u,v) \text{ is continuous on } \mathcal{V} \text{ for the norm of } \mathsf{H}\big\}\,,$$

satisfies the following properties:

(i) *$\mathscr{L}$ is bijective from $\mathsf{Dom}(\mathscr{L})$ onto H,*

(ii) *$\mathsf{Dom}(\mathscr{L})$ is dense in $\mathcal{V}$ and in H,*

(iii) *$\mathscr{L}$ is closed.*

18.3.2 Weighted coercivity estimates

For any complex number μ, consider the shifted form $Q_\mu(u,v) := Q(u,v) - \mu\,\langle u, v\rangle$. The aim of this subsection is to prove the following estimate and deduce Theorem 18.1 from it (with help of Theorem 18.6).

Theorem 18.7 (Weighted coercivity)**.** *For every $\mu \in \mathbb{C}$, $W \in W^{1,\infty}(\Omega;\mathbb{R})$ and all $u \in \mathcal{C}_0^\infty(\Omega)$, we have*

$$\begin{aligned}\Re\big[Q_\mu(u, e^{2W}u)\big] + \Im\big[Q_\mu(u, \Phi e^{2W}u)\big] \geq \frac{1}{2}\,\big\|(-i\nabla + \mathbf{A})e^W u\big\|^2 \\ + \int_\Omega |e^W u|^2 \Bigg[\frac{V_2^2 + \frac{1}{12d}|\mathbf{B}|^2}{m_{\mathbf{B},V}} + V_1 - \Re\mu - |\Im\mu| \\ - 9\left(|\nabla\Phi|^2 + |\nabla\Psi|^2 + |\nabla W|^2\right)\Bigg]\,\mathrm{d}x\,.\end{aligned}$$

In order to prove Theorem 18.7, we need two lemmata.

Lemma 18.1. *For every $u \in \mathcal{C}_0^\infty(\Omega)$, we have*

$$\int_\Omega \frac{|\mathbf{B}|^2}{m_{\mathbf{B},V}} |u|^2 \, \mathrm{d}x \leq 3d \, \|(-i\nabla + \mathbf{A})u\|^2 + \|(\nabla\Psi)u\|^2 \, .$$

Proof. Let $u \in \mathcal{C}_0^\infty(\Omega)$ and $j,k \in [\![1,d]\!] := [1,d] \cap \mathbb{Z}$. Using (18.7) and (18.8), we have

$$\begin{aligned}\int_\Omega \frac{B_{jk}^2}{m_{\mathbf{B},V}} |u|^2 \, \mathrm{d}x &= \langle i[P_j,P_k]u, \Psi_{jk}u\rangle = \langle iP_k u, P_j\Psi_{jk}u\rangle - \langle iP_j u, P_k \Psi_{jk} u\rangle \\ &= \langle iP_k u, \Psi_{jk}P_j u\rangle - \langle iP_j u, \Psi_{jk}P_k u\rangle - \langle P_k u, (\partial_j \Psi_{jk})u\rangle + \langle P_j u, (\partial_k \Psi_{jk})u\rangle \\ &\leq \frac{3}{2}\|P_j u\|^2 + \frac{3}{2}\|P_k u\|^2 + \frac{1}{2}\|(\partial_j\Psi_{jk})u\|^2 + \frac{1}{2}\|(\partial_k \Psi_{jk})u\|^2 \, .\end{aligned}$$

We conclude by summing over $j,k \in [\![1,d]\!]$. □

The second lemma follows elementarily by a commutator computation.

Lemma 18.2. *For every $u \in \mathcal{C}_0^\infty(\Omega)$ and $\chi \in W^{1,\infty}(\Omega;\mathbb{R})$, we have*

$$\Re \langle (-i\nabla + \mathbf{A})u, (-i\nabla + \mathbf{A})\chi^2 u\rangle = \|(-i\nabla + \mathbf{A})\chi u\|^2 - \|(\nabla\chi)u\|^2 \, .$$

Now we are in a position to prove Theorem 18.7.

Proof of Theorem 18.7. Let us consider $u \in \mathcal{C}_0^\infty(\Omega)$ and $W \in W^{1,\infty}(\Omega;\mathbb{R})$. Choosing $\chi := e^W$ in Lemma 18.2, we get the identity

$$\Re\big[Q(u, e^{2W}u)\big] = \int_\Omega V_1 |e^W u|^2 \, \mathrm{d}x + \big\|(-i\nabla + \mathbf{A})e^W u\big\|^2 - \big\|(\nabla W)e^W u\big\|^2 \, . \tag{18.21}$$

Moreover, we have

$$\begin{aligned}&\Im\big[Q(u, \Phi e^{2W}u)\big] \\ &\qquad = \Im \langle (-i\nabla + \mathbf{A})u, (-i\nabla + \mathbf{A})(\Phi e^{2W}u)\rangle + \int_\Omega \frac{V_2^2}{m_{\mathbf{B},V}} |e^W u|^2 \, \mathrm{d}x \, .\end{aligned}$$

The first term of the right-hand side equals

$$\begin{aligned}&\Im \langle (-i\nabla + \mathbf{A})u, -i(\nabla\Phi + 2\Phi\nabla W)e^{2W}u)\rangle \\ &\quad = \Im \langle e^W(-i\nabla + \mathbf{A})u, -i(\nabla\Phi + 2\Phi\nabla W)e^W u)\rangle \\ &\quad = \Im \langle (-i\nabla + \mathbf{A})e^W u, -i(\nabla\Phi + 2\Phi\nabla W)e^W u)\rangle \, .\end{aligned}$$

Consequently, for all $\alpha \in (0,1)$, we have

$$\begin{aligned}&|\Im \langle (-i\nabla + \mathbf{A})u, (-i\nabla + \mathbf{A})(\Phi e^{2W}u)\rangle| \\ &\qquad \leq \alpha \big\|(-i\nabla + \mathbf{A})e^W u\big\|^2 + \frac{1}{4\alpha}\big\|\big(\nabla\Phi + 2(\nabla W)\Phi\big)e^W u\big\|^2\end{aligned}$$

and therefore

$$\begin{aligned}\Im\big[Q(u, \Phi e^{2W}u)\big] \geq &\int_\Omega \frac{V_2^2}{m_{\mathbf{B},V}} |e^W u|^2 \, \mathrm{d}x \\ &- \alpha \big\|(-i\nabla + \mathbf{A})e^W u\big\|^2 - \frac{1}{4\alpha}\big\|\big(\nabla\Phi + 2(\nabla W)\Phi\big)e^W u\big\|^2 \, .\end{aligned} \tag{18.22}$$

Summing up (18.21) and (18.22), we deduce

$$\begin{aligned}\Re\big[Q(u, e^{2W}u)\big] + \Im\big[Q(u, \Phi e^{2W}u)\big] &\geq (1-\alpha)\big\|(-i\nabla + \mathbf{A})e^W u\big\|^2 \\ &+ \int_\Omega |e^W u|^2 \left(\frac{V_2^2}{m_{\mathbf{B},V}} + V_1 - |\nabla W|^2 - \frac{1}{2\alpha}|\nabla\Phi|^2 - \frac{2}{\alpha}|\nabla W|^2\right) \mathrm{d}x \, .\end{aligned}$$

It remains to add the term involving $|\mathbf{B}|^2$. By Lemma 18.1, we have

$$\left\|(-i\nabla+\mathbf{A})e^W u\right\|^2 \geq \frac{1}{3d}\left(\int_\Omega \frac{|\mathbf{B}|^2}{m_{\mathbf{B},V}}|e^W u|^2\,\mathrm{d}x - \left\|(\nabla\Psi)e^W u\right\|^2\right).$$

Thus, for all $\beta\in[0,1-\alpha]$, we get

$$\begin{aligned}\Re\big[Q(u,e^{2W}u)\big] + \Im\big[Q(u,\Phi e^{2W}u)\big] &\geq (1-\alpha-\beta)\left\|(-i\nabla+\mathbf{A})e^W u\right\|^2 \\ &+ \int_\Omega |e^W u|^2\left[\frac{V_2^2+\frac{\beta}{3d}|\mathbf{B}|^2}{m_{\mathbf{B},V}} + V_1 - \frac{2+\alpha}{\alpha}|\nabla W|^2 - \frac{1}{2\alpha}|\nabla\Phi|^2 - \frac{\beta}{3d}|\nabla\Psi|^2\right]\mathrm{d}x\,.\end{aligned}$$

The proof is concluded by taking $\alpha=\beta=\frac14$ and adding the contribution related to the shift by μ. ☐

With Theorems 18.6 and 18.7 we easily deduce Theorem 18.1.

Proof of Theorem 18.1. Under Assumption 18.1, the inequality of Theorem 18.7 extends to all $u\in\mathscr{V}$. Applied with $W=0$, Theorem 18.7 then gives, for all $u\in\mathscr{V}$,

$$\begin{aligned}|Q_\mu(u,u)| + |Q_\mu(u,\Phi u)| &\geq \frac12\left\|(-i\nabla+\mathbf{A})u\right\|^2 \\ &+ \int_\Omega |u|^2\left(\frac{V_2^2+\frac{1}{12d}|B|^2}{m_{\mathbf{B},V}} + V_1 - \Re\mu - |\Im\mu| - 9(|\nabla\Phi|^2+|\nabla\Psi|^2)\right)\mathrm{d}x\,.\end{aligned} \tag{18.23}$$

Using Assumption 18.1, it implies

$$\begin{aligned}|Q_\mu(u,u)| + |Q_\mu(u,\Phi u)| &\geq \frac12\left\|(-i\nabla+\mathbf{A})u\right\|^2 \\ &+ \int_\Omega \left(\gamma_1 m_{\mathbf{B},V} - \Re\mu - |\Im\mu| - \gamma_2\right)|u|^2\,\mathrm{d}x\,.\end{aligned} \tag{18.24}$$

Taking $\mu\in\mathbb{R}$ such that $\mu<-\gamma_2$, the inequality establishes the coercivity of Q_μ on $\mathscr{V}$, so it is enough to apply Theorem 18.6 to Q_μ. ☐

18.3.3 Description of the operator domain

At this moment, we only know that the operator domain of $\mathscr{L}$ is given by (18.14). This subsection is devoted to a proof of Theorem 18.2, which gives a more explicit characterisation of $\mathsf{D}(\mathscr{L})$.

Let us first state a density result.

Lemma 18.3. *The set*

$$\mathcal{D} := \left\{u\in\mathsf{Dom}(\mathscr{L})\ :\ \operatorname{supp} u \ \ \textit{is compact in } \overline{\Omega}\right\} \tag{18.25}$$

is a core of $\mathscr{L}$.

Proof. From the definition of $\mathsf{Dom}(\mathscr{L})$ given by (18.14), we get that

$$\mathsf{Dom}(\mathscr{L}) \subset \{u\in\mathscr{V}\ :\ (-i\nabla+\mathbf{A})^2u + Vu \in L^2(\Omega)\}\,. \tag{18.26}$$

Take $u\in\mathsf{Dom}(\mathscr{L})$ and notice that $Vu\in L^2_{\mathrm{loc}}(\overline{\Omega})$ from our regularity assumption about V, thus $(-i\nabla+\mathbf{A})^2u\in L^2_{\mathrm{loc}}(\overline{\Omega})$ as well. We define a suitable cut-off, see [10, proof of Thm. 8.2.1]. Consider a non-negative function $\varphi\in\mathcal{C}_0^\infty(\mathbb{R}^d)$ such that $\varphi(x)=1$ if $|x|<1$ and $\varphi(x)=0$ if $|x|>2$ and, for $u\in\mathsf{Dom}(\mathscr{L})$, define, for all $x\in\Omega$ and $n\in\mathbb{N}$,

$$u_n(x) := u(x)\varphi_n(x)\,, \qquad \varphi_n(x) := \varphi\left(\frac{x}{n}\right). \tag{18.27}$$

Since

$$(-i\nabla+\mathbf{A})^2u_n = \varphi_n(-i\nabla+\mathbf{A})^2u - 2i\nabla\varphi_n\cdot(-i\nabla+\mathbf{A})u - (\Delta\varphi_n)u\,, \tag{18.28}$$

we have from the derived regularity of u and the compactness of $\operatorname{supp}\varphi_n$ that $\{u_n\}_{n\in\mathbb{N}}\subset\mathcal{D}$. Moreover, by the dominated convergence theorem, $\|u_n-u\|\to0$ as $n\to\infty$ and

$$\begin{aligned}&\|[(-i\nabla+\mathbf{A})^2+V]u - [(-i\nabla+\mathbf{A})^2+V]u_n\| \\ &\qquad\leq \|(1-\varphi_n)[(-i\nabla+\mathbf{A})^2+V]u\| + 2\|\nabla\varphi_n\cdot(-i\nabla+\mathbf{A})u\| + \|(\Delta\varphi_n)u\| \xrightarrow[n\to\infty]{} 0\,,\end{aligned}$$

since $\|\nabla\varphi_n\|_{L^\infty(\mathbb{R}^d)} = n^{-1}\|\nabla\varphi\|_{L^\infty(\mathbb{R}^d)}$, $\|\Delta\varphi_n\|_{L^\infty(\mathbb{R}^d)} = n^{-2}\|\Delta\varphi\|_{L^\infty(\mathbb{R}^d)}$ and $u\in\mathscr{V}$. ☐

By integrating by parts, we get the following lemma.

Lemma 18.4. *For all $u \in \mathcal{D}$ and $\delta > 0$, we have*

$$2\,\|(-i\nabla + \mathbf{A})u\|^2 \leq \delta\|(-i\nabla + \mathbf{A})^2 u\|^2 + \delta^{-1}\|u\|^2\,.$$

Proof. For every $u \in \mathcal{D}$, we have

$$\|(-i\nabla + \mathbf{A})u\|^2 = \langle(-i\nabla + \mathbf{A})u, (-i\nabla + \mathbf{A})u\rangle = \big\langle(-i\nabla + \mathbf{A})^2 u, u\big\rangle$$

where the second equality employs an integration by parts using our regularity assumptions about V and $\mathbf{A}$, namely $Vu \in L^2(\Omega)$ with (18.26). The proof is concluded by applying the Cauchy-Schwarz and Young inequalities. □

In the following Lemma 18.5 and Proposition 18.3, we establish estimates on $|\mathbf{B}|u$; the proofs are adaptations of [4, Lem. 3.4].

Lemma 18.5. *Suppose* (18.11)*. There exists $C > 0$ such that, for all $u \in \mathcal{D}$,*

$$\big\||\mathbf{B}|u\big\|^2 \leq C\left(\|m_{\mathbf{B},V}^{\frac{1}{2}}(-i\nabla + \mathbf{A})u\|^2 + \|Vu\|^2 + \|(-i\nabla + \mathbf{A})^2 u\|^2 + \|u\|^2\right)\,. \tag{18.29}$$

Proof. Let $u \in \mathcal{D}$. Then $B_{jk}u \in \mathscr{V}$ and similarly as in Lemma 18.1, we have

$$\|B_{jk}u\|^2 = \Im\langle[P_j, P_k]u, B_{jk}u\rangle \leq |\langle P_k u, P_j B_{jk}u\rangle| + |\langle P_j u, P_k B_{jk}u\rangle| \tag{18.30}$$

for every $j, k \in [\![1, d]\!]$. Further, using the assumption (18.11), we get that, for all $\varepsilon_1 > 0$, there exist $C_{\varepsilon_1}, \tilde{C}_{\varepsilon_1} > 0$ such that

$$\begin{aligned}
|\langle P_k u, P_j B_{jk}u\rangle| &\leq |\langle B_{jk}P_k u, P_j u\rangle| + |\langle P_k u, u\partial_j B_{jk}\rangle| \\
&\leq \||B_{jk}|^{\frac{1}{2}}P_k u\|\,\||B_{jk}|^{\frac{1}{2}}P_j u\| + \varepsilon_1\|m_{\mathbf{B},V}^{\frac{1}{2}}P_k u\|\,\|m_{\mathbf{B},V}u\| \\
&\quad + C_{\varepsilon_1}\|P_k u\|\,\|u\| \\
&\leq \||B_{jk}|^{\frac{1}{2}}P_k u\|\,\||B_{jk}|^{\frac{1}{2}}P_j u\| + \\
&\quad + \varepsilon_1\left(\|m_{\mathbf{B},V}^{\frac{1}{2}}P_k u\|^2 + \|m_{\mathbf{B},V}u\|^2 + \|P_k u\|^2\right) + \tilde{C}_{\varepsilon_1}\|u\|^2\,.
\end{aligned} \tag{18.31}$$

Summing up over j and k, we get from (18.30) and (18.31) that there exists $C_1 > 0$ such that, for all $\varepsilon_1 \in (0,1)$, there exists $\hat{C}_{\varepsilon_1} > 0$ such that

$$\||\mathbf{B}|u\|^2 \leq C_1\left(\|m_{\mathbf{B},V}^{\frac{1}{2}}(-i\nabla + \mathbf{A})u\|^2 + \varepsilon_1\big(\|m_{\mathbf{B},V}u\|^2 + \|(-i\nabla + \mathbf{A})u\|^2\big)\right) + \hat{C}_{\varepsilon_1}\|u\|^2\,.$$

We now use Lemma 18.4 to get the desired estimate. □

Proposition 18.3. *Suppose* (18.11)*. There exists $C > 0$, such that, for all $u \in \mathcal{D}$, we have*

$$\||\mathbf{B}|u\|^2 + \|m_{\mathbf{B},V}^{\frac{1}{2}}(-i\nabla + \mathbf{A})u\|^2 \leq C\left(\|(-i\nabla + \mathbf{A})^2 u\|^2 + \|Vu\|^2 + \|u\|^2\right)\,. \tag{18.32}$$

Proof. Let us first show that, for all $\varepsilon > 0$, there exists $C_\varepsilon > 0$ such that, for all $u \in \mathcal{D}$,

$$\|m_{\mathbf{B},V}^{\frac{1}{2}}(-i\nabla + \mathbf{A})u\|^2 \leq C_\varepsilon(\|(-i\nabla + \mathbf{A})^2 u\|^2 + \|u\|^2) + \varepsilon\|m_{\mathbf{B},V}u\|^2\,. \tag{18.33}$$

We write

$$\|m_{\mathbf{B},V}^{\frac{1}{2}}(-i\nabla + \mathbf{A})u\|^2 = \langle m_{\mathbf{B},V}(-i\nabla + \mathbf{A})u, (-i\nabla + \mathbf{A})u\rangle\,,$$

so that, by an integration by parts,

$$\|m_{\mathbf{B},V}^{\frac{1}{2}}(-i\nabla + \mathbf{A})u\|^2 = \langle(-i\nabla m_{\mathbf{B},V})(-i\nabla + \mathbf{A})u, u\rangle + \langle m_{\mathbf{B},V}(-i\nabla + \mathbf{A})^2 u, u\rangle\,. \tag{18.34}$$

We have, for all $\varepsilon_1 \in (0,1)$,

$$|\langle m_{\mathbf{B},V}(-i\nabla + \mathbf{A})^2 u, u\rangle| \leq \frac{\varepsilon_1}{2}\|m_{\mathbf{B},V}u\|^2 + \frac{1}{2\varepsilon_1}\|(-i\nabla + \mathbf{A})^2 u\|^2\,. \tag{18.35}$$

Moreover, by using (18.11) and Lemma 18.4, for all $\varepsilon_1 \in (0,1)$, there exists $C_{\varepsilon_1} > 0$ such that

$$|\langle(-i\nabla m_{\mathbf{B},V})(-i\nabla+\mathbf{A})u,u\rangle| \leq \frac{\varepsilon_1}{2}\left(\|m_{\mathbf{B},V}^{\frac{1}{2}}(-i\nabla+\mathbf{A})u\|^2 + \|m_{\mathbf{B},V}u\|^2\right) + C_{\varepsilon_1}\left(\|u\|^2 + \|(-i\nabla+\mathbf{A})^2u\|^2\right) . \quad (18.36)$$

Using (18.34), (18.35) and (18.36), we deduce (18.33). Having established (18.33), it remains to combine it with Lemma 18.5 and choose ε sufficiently small. □

Now we are in a position to establish Theorem 18.2.

Proof of Theorem 18.2. For all $u \in \mathcal{D}$, we have

$$\begin{aligned}\|\mathscr{L}u\|^2 &= \|(-i\nabla+\mathbf{A})^2u\|^2 + \|Vu\|^2 + 2\Re\langle(-i\nabla+\mathbf{A})^2u, Vu\rangle \\ &= \|(-i\nabla+\mathbf{A})^2u\|^2 + \|Vu\|^2 + 2\Re\langle(-i\nabla+\mathbf{A})u, (-i\nabla+\mathbf{A})(Vu)\rangle \\ &\geq \|(-i\nabla+\mathbf{A})^2u\|^2 + \|Vu\|^2 + 2\int_\Omega V_1|(-i\nabla+\mathbf{A})u|^2\,\mathrm{d}x \\ &\quad - 2\langle|(-i\nabla+\mathbf{A})u|, |\nabla V||u|\rangle\,.\end{aligned} \quad (18.37)$$

Note that the second step is justified since $Vu \in \mathscr{V}$. We proceed by estimating the last term of (18.37). Let $\varepsilon \in (0,1)$. There exist $C_\varepsilon, \tilde{C}_\varepsilon > 0$ such that

$$\begin{aligned}&2\langle|(-i\nabla+\mathbf{A})u|, |\nabla V||u|\rangle \\ &\quad\leq 2\varepsilon\langle|(-i\nabla+\mathbf{A})u|, m_{\mathbf{B},V}^{\frac{3}{2}}|u|\rangle + 2C_\varepsilon\langle|(-i\nabla+\mathbf{A})u|, |u|\rangle \\ &\quad\leq 2\varepsilon(\|m_{\mathbf{B},V}^{\frac{1}{2}}(-i\nabla+\mathbf{A})u\|^2 + \|m_{\mathbf{B},V}u\|^2) + \tilde{C}_\varepsilon\|u\|^2\,.\end{aligned} \quad (18.38)$$

From (18.37), (18.38), (18.12) and Lemma 18.4, we deduce that, for some $\hat{C}_\varepsilon > 0$,

$$\begin{aligned}\|\mathscr{L}u\|^2 \geq (1-2\varepsilon)&\left(\|(-i\nabla+\mathbf{A})^2u\|^2 + \|Vu\|^2\right) - 2\varepsilon\||\mathbf{B}|u\|^2 \\ &- 3\varepsilon\|m_{\mathbf{B},V}^{\frac{1}{2}}(-i\nabla+\mathbf{A})u\|^2 - \hat{C}_\varepsilon\|u\|^2\,.\end{aligned} \quad (18.39)$$

Finally, using Proposition 18.3, we get

$$\|\mathscr{L}u\|^2 \geq (1-2\varepsilon-3C\varepsilon)\left(\|(-i\nabla+\mathbf{A})^2u\|^2 + \|Vu\|^2\right) - (\hat{C}_\varepsilon + 3C\varepsilon)\|u\|^2\,. \quad (18.40)$$

The claim follows by the density of $\mathcal{D}$ in $\mathsf{Dom}(\mathscr{L})$, see Lemma 18.3. □

18.3.4 On Assumption 18.1

We conclude this section by establishing the sufficient condition of Proposition 18.1. Note that Theorem 18.1 is proved under Assumption 18.1, while our proof of Theorem 18.2 requires the stronger hypotheses (18.11) and (18.12).

Proof of Proposition 18.1. The proof follows from the fact that, by (18.11),

$$|\nabla\Phi(x)|^2 + |\nabla\Psi(x)|^2 \underset{|x|\to+\infty}{=} o(m_{\mathbf{B},V}(x))\,.$$

Indeed, using in addition (18.12), we may write

$$\begin{aligned}&\frac{V_2^2 + \frac{1}{12d}|\mathbf{B}|^2}{m_{\mathbf{B},V}} + V_1 - 9\left(|\nabla\Phi|^2 + |\nabla\Psi|^2\right) \\ &\quad\geq \frac{1}{12d}\frac{|V|^2 + |\mathbf{B}|^2}{m_{\mathbf{B},V}} + V_1 - \frac{V_1^2}{m_{\mathbf{B},V}} - 9\left(|\nabla\Phi|^2 + |\nabla\Psi|^2\right) \\ &\quad\geq \frac{1}{12d}m_{\mathbf{B},V} - \frac{1}{12d} + o(m_{\mathbf{B},V})\,,\end{aligned}$$

which provides (18.9). □

18.4 Discrete spectrum and exponential estimates of eigenfunctions

The main objective of this section is to establish Proposition 18.2 and Theorems 18.3 and 18.4.

18.4.1 Confining potentials

In addition to Assumption 18.1, let us assume that V is confining in the sense of (18.16).

Proof of Proposition 18.2. By Theorem 18.1, we already know that the resolvent of $\mathscr{L}$ exists at a point of the complex plane. Hence, it is enough to show that $\mathsf{D}(\mathscr{L})$ is compactly embedded in $L^2(\Omega)$. Consider (18.24) with $\mu = 0$. By the definition of $\mathscr{L}$ given in (18.13) and the Cauchy-Schwarz inequality, we get

$$\int_\Omega (\gamma_1 m_{\mathbf{B},V} - \gamma_2)|u|^2 \,\mathrm{d}x \leq 2\|\mathscr{L}u\|\|u\| \leq \|\mathscr{L}u\|^2 + \|u\|^2 =: \|u\|_{\mathscr{L}}^2$$

for all $u \in \mathsf{Dom}(\mathscr{L})$. Moreover, we have $\mathsf{Dom}(\mathscr{L}) \subset H^2_{\mathsf{loc}}(\Omega)$. Thus, by the Riesz-Fréchet-Kolmogorov criterion, the unit ball for the graph norm of $\mathscr{L}$ is precompact in $L^2(\Omega)$ and thus $\mathscr{L}$ is an operator with compact resolvent. □

18.4.2 General potentials

Now let us assume only Assumption 18.1.

Proof of Theorem 18.3. The inclusion (18.17) is again a consequence of (18.24) and Theorem 18.6. It is sufficient to prove (18.18). Let $\mu \in \rho_{\gamma_2 - \gamma_1 \check{m}_\infty}$. Of course, if $\mu \in \rho_{\gamma_2}$ there is nothing to prove. Let us define $R > 0$ such that,

$$\forall |x| \geq R\,, \qquad m_{\mathbf{B},V}(x) \geq \check{m}_\infty\,. \tag{18.41}$$

Then, we have

$$\gamma_1 m_{\mathbf{B},V}(x) - \Re\mu - |\Im\mu| - \gamma_2 \geq \gamma_1 \check{m}_\infty - \Re\mu - |\Im\mu| - \gamma_2 =: \gamma > 0 \tag{18.42}$$

for all $|x| \geq R$. Let us introduce a real-valued smooth function with compact support $0 \leq \chi \leq 1$ such that $\chi(x) = 0$ for all $|x| \geq 2R$ and $\chi(x) = 1$ for all $|x| \leq R$. We define

$$M := |\gamma_2 + \Re\mu + |\Im\mu|| + 1 \in [1, +\infty)\,.$$

Let us write

$$\mathscr{L} - \mu = \mathscr{L} + M\chi - \mu - M\chi\,.$$

We introduce the (closed) operator $\widetilde{\mathscr{L}} := \mathscr{L} + M\chi$ and, for $\mu \in \mathbb{C}$, the corresponding shifted form $\widetilde{Q}_\mu := Q_\mu + M\chi$.

Let us explain why $\widetilde{\mathscr{L}} - \mu$ is invertible. For that purpose, we recall that by Theorem 18.7 (with $W = 0$) and Assumption 18.1, we have, for all $u \in \mathscr{V}$,

$$\begin{aligned}\Re\big[\widetilde{Q}_\mu(u,u)\big] &+ \Im\big[\widetilde{Q}_\mu(u,\Phi u)\big] \\ &\geq \frac{1}{2}\,\|(-i\nabla + \mathbf{A})u\|^2 + \int_\Omega \big(M\chi + \gamma_1 m_{\mathbf{B},V} - \gamma_2 - \Re\mu - |\Im\mu|\big)|u|^2 \,\mathrm{d}x\,.\end{aligned}$$

By the definitions of M and γ, we deduce that

$$\Re\big[\widetilde{Q}_\mu(u,u)\big] + \Im\big[\widetilde{Q}_\mu(u,\Phi u)\big] \geq \frac{1}{2}\,\|(-i\nabla + \mathbf{A})u\|^2 + \min(1,\gamma)\,\|u\|^2\,.$$

This proves the coercivity of $\widetilde{Q}_\mu$ on $\mathscr{V}$ and thus, by Theorem 18.6, $\widetilde{\mathscr{L}} - \mu$ is invertible.

Now, the multiplication operator $M\chi$ is a relatively compact perturbation of $\widetilde{\mathscr{L}} - \mu$. Therefore, by Lemma 18.7, $\mathscr{L} - \mu$ is a Fredholm operator with index 0. From Lemma 18.8, we deduce that the spectrum in $\rho_{\gamma_2 - \gamma_1 \check{m}_\infty}$ is discrete (that is, made of isolated eigenvalues of finite algebraic multiplicity, see Appendix 18.5).

This concludes the proof of the theorem. □

18.4.3 Agmon-type estimates

Theorem 18.4 is essentially a consequence of the following proposition about properties of solutions of an inhomogeneous equation in a weighted space.

Proposition 18.4. *Let $\lambda \in \mathsf{sp}(\mathscr{L}) \cap \rho_{\gamma_2-\gamma_1 \check{m}_\infty} \neq \emptyset$. Let us consider $\psi_0 \in L^2(\Omega)$ such that*

$$e^{\frac{1-\varepsilon}{3}\,\mathrm{d}_{\mathsf{Ag}}(x)}\psi_0 \in L^2(\Omega) \tag{18.43}$$

for some $\varepsilon \in (0,1)$ and assume that $\psi \in \mathsf{Dom}(\mathscr{L})$ satisfies

$$\mathscr{L}\psi = \lambda\psi + \psi_0\,. \tag{18.44}$$

Then

$$e^{\frac{1-\varepsilon}{3}\,\mathrm{d}_{\mathsf{Ag}}(x)}\psi \in L^2(\Omega)\,. \tag{18.45}$$

Proof. By Theorem 18.3, λ is an eigenvalue of finite algebraic multiplicity. Given $W \in W^{1,\infty}(\Omega;\mathbb{R})$, we have

$$\begin{aligned}\Re Q(\psi, e^{2W}\psi) &= \Re(\lambda)\|e^W\psi\|^2 + \Re\left\langle e^W\psi_0, e^W\psi\right\rangle\,,\\ \Im Q(\psi, \Phi e^{2W}\psi) &= \Im(\lambda)\int_\Omega \Phi e^{2W}|\psi|^2\,\mathrm{d}x + \Im\left\langle e^W\psi_0, \Phi e^W\psi\right\rangle\,.\end{aligned}$$

By Theorem 18.7 (with $\mu = 0$) and Assumption 18.1,

$$\begin{aligned}&\left(\Re(\lambda) + |\Im(\lambda)|\right)\left\|e^W\psi\right\|^2\\ &\qquad\geq \int_\Omega \left(\gamma_1 m_{\mathbf{B},V} - \gamma_2 - 9|\nabla W|^2\right)|e^W\psi|^2\,\mathrm{d}x - \left\|e^W\psi_0\right\|\left\|e^W\psi\right\|\,.\end{aligned}$$

Thus, we get

$$\begin{aligned}&\int_\Omega \left(\gamma_1 m_{\mathbf{B},V} - \Re(\lambda) - |\Im(\lambda)| - \gamma_2 - 9|\nabla W|^2\right)|e^W\psi|^2\,\mathrm{d}x\\ &\qquad\leq \left\|e^W\psi_0\right\|\left\|e^W\psi\right\|\,.\end{aligned}$$

Let R be as in (18.41). Splitting the integral into two parts, we get

$$\begin{aligned}&\int_{\{|x|>R\}} \left(\gamma_1 m_{\mathbf{B},V} - \Re(\lambda) - |\Im(\lambda)| - \gamma_2 - 9|\nabla W|^2\right)|e^W\psi|^2\,\mathrm{d}x\\ &\quad\leq \int_{\{|x|<R\}} \left(-\gamma_1 m_{\mathbf{B},V} + \Re(\lambda) + |\Im(\lambda)| + \gamma_2 + 9|\nabla W|^2\right)|e^W\psi|^2\,\mathrm{d}x\\ &\qquad + \left\|e^W\psi_0\right\|\left\|e^W\psi\right\|\,,\end{aligned}$$

so that, for some $C > 0$, we have by (18.19),

$$\begin{aligned}&\int_{\{|x|>R\}} \left(|\nabla \mathrm{d}_{\mathsf{Ag}}(x)|^2 - 9|\nabla W|^2\right)|e^W\psi|^2\,\mathrm{d}x\\ &\qquad\leq \int_{\{|x|<R\}} \left(C + 9|\nabla W|^2\right)|e^W\psi|^2\,\mathrm{d}x + \left\|e^W\psi_0\right\|\left\|e^W\psi\right\|\,.\end{aligned} \tag{18.46}$$

We set $\eta := \frac{\sqrt{1-\varepsilon}}{3}$ and we consider the functions $(\chi_n)_{n\geq 1}$ defined as follows

$$\chi_n(s) := \begin{cases} s & \text{for } 0 \leq s \leq n\,,\\ 2n - s & \text{for } n \leq s \leq 2n\,,\\ 0 & \text{for } s \geq 2n\,. \end{cases}$$

Note that $|\chi_n'(s)| = 1$ a.e. on $[0, 2n]$ and $|\chi_n'(s)| = 0$ for $s > 2n$.

Then for $n \geq 1$ and $x \in \Omega$ we set

$$W_n(x) := \eta\,\chi_n(\mathrm{d}_{\mathsf{Ag}}(x))\,.$$

We have

$$\nabla W_n(x) = \eta\,\chi_n'(\mathrm{d}_{\mathsf{Ag}}(x))\nabla \mathrm{d}_{\mathsf{Ag}}(x)$$

and

$$|\nabla W_n(x)|^2 \leq \eta^2|\nabla \mathrm{d}_{\mathsf{Ag}}(x)|^2 = \frac{1-\varepsilon}{9}|\nabla \mathrm{d}_{\mathsf{Ag}}(x)|^2\,.$$

By (18.46) we obtain that there exists $C>0$ such that, for all $n\geq 1$,

$$\int_{\{|x|>R\}} \varepsilon|\nabla \mathrm{d}_{\mathsf{Ag}}(x)|^2|e^{W_n}\psi|^2\,\mathrm{d}x \leq C\|\psi\|^2 + \left\|e^{W_n}\psi\right\|\left\|e^{W_n}\psi_0\right\|\,,$$

and therefore, by (18.42),

$$\int_{\{|x|>R\}} \varepsilon\gamma|e^{W_n}\psi|^2\,\mathrm{d}x \leq C\|\psi\|^2 + \frac{\varepsilon\gamma}{2}\left\|e^{W_n}\psi\right\|^2 + \frac{1}{2\varepsilon\gamma}\left\|e^{W_n}\psi_0\right\|^2\,.$$

For another constant $C>0$ independent of n, we get

$$\int_\Omega |e^{W_n}\psi|^2\,\mathrm{d}x \leq C\|\psi\|^2 + C\left\|e^{W_n}\psi_0\right\|^2\,.$$

It remains to take the limit $n\to+\infty$ and use the Fatou lemma to conclude. □

Now we are in a position to prove the main result of this paper.

Proof of Theorem 18.4. If $\psi\in\mathsf{N}(\mathscr{L}-\lambda)$, we apply Proposition 18.4 with $\psi_0=0$ to deduce that ψ satisfies (18.20).

Let us now explain why this conclusion holds also for the algebraic eigenspace (see Appendix 18.5). Let us consider ψ in this space.

We have

$$(\mathscr{L}-\lambda)^r\psi = 0 \qquad \text{with} \qquad r := \dim \mathsf{R}(P_\lambda)\geq 1\,.$$

Now, we proceed by induction. Consider $k\in[\![1,r]\!]$ and assume that

$$(\mathscr{L}-\lambda)^k\psi \in L^2\left(\Omega, e^{\frac{1-\varepsilon}{3}\mathrm{d}_{\mathsf{Ag}}(x)}\,\mathrm{d}x\right)\,.$$

Then, we write

$$(\mathscr{L}-\lambda)\left\{(\mathscr{L}-\lambda)^{k-1}\psi\right\} = (\mathscr{L}-\lambda)^k\psi\,.$$

We are in the situation (18.44) and we deduce that

$$(\mathscr{L}-\lambda)^{k-1}\psi \in L^2\left(\Omega, e^{\frac{1-\varepsilon}{3}\mathrm{d}_{\mathsf{Ag}}(x)}\,\mathrm{d}x\right)\,.$$

This concludes the proof. □

18.5 Appendix: Reminders of spectral theory

Since spectral theory of non-self-adjoint operators is less unified than its self-adjoint sister, in this appendix we collect some notions used throughout the paper. We refer to standard monographs [21], [13, Chap. I.3, IX] and [18, Chap. XVII] or a recent summary [22] for a more comprehensive exposition.

Let H be a Hilbert space. An operator $\mathscr{M}:\mathsf{Dom}(\mathscr{M})\to\mathsf{H}$ is said to be *Fredholm* when $\mathsf{N}(\mathscr{M})$ finite-dimensional and $\mathsf{R}(\mathscr{M})$ is closed with finite codimension. Then the *index* of $\mathscr{M}$ is defined by $\operatorname{ind}(\mathscr{M}) := \dim\mathsf{N}(\mathscr{M}) - \operatorname{codim}\mathsf{R}(\mathscr{M})$. When $\mathsf{Dom}(\mathscr{M})$ is dense in H, we may classically define the adjoint $\mathscr{M}^*$ of $\mathscr{M}$ and then we have $\dim\mathsf{N}(\mathscr{M}^*) = \operatorname{codim}\mathsf{R}(\mathscr{M})$. We denote by $\mathsf{Fred}_0(\mathscr{M})$ the set of all complex numbers λ such that $\mathscr{M}-\lambda$ is a Fredholm operator with index 0.

Let $\mathscr{M}$ be an arbitrary closed operator in H. The *spectrum* $\mathsf{sp}(\mathscr{M})$ is defined as the set of all complex numbers λ such that $\mathscr{M}-\lambda$ is not bijective as an operator from $\mathsf{D}(\mathscr{M})$ to H. The *resolvent set* $\rho(\mathscr{M})$ is the complement of the spectrum in the complex plane. We call the intersection $\mathsf{sp}_{\mathsf{fre}}(\mathscr{M}) := \mathsf{sp}(\mathscr{M})\cap\mathsf{Fred}_0(\mathscr{M})$ the *Fredholm spectrum* and define the *essential spectrum* by the complement $\mathsf{sp}_{\mathsf{ess}}(\mathscr{M}) := \mathsf{sp}(\mathscr{M})\setminus\mathsf{sp}_{\mathsf{fre}}(\mathscr{M})$ (it is the essential spectrum due to Schechter denoted by $\mathsf{sp}_{\mathsf{e4}}(\mathscr{M})$ in [13]). Finally, we define the *discrete spectrum* $\mathsf{sp}_{\mathsf{dis}}(\mathscr{M})$ to be the set of all isolated eigenvalues λ for which the *algebraic* (or *root*) eigenspace $\bigcup_{k=1}^\infty \mathsf{N}([\mathscr{M}-\lambda]^k)$ is finite-dimensional and such that $\mathscr{M}-\lambda$ has a closed range. The elements of $\mathsf{sp}_{\mathsf{dis}}(\mathscr{M})$ are called the *discrete eigenvalues* of $\mathscr{M}$.

Let λ be an isolated eigenvalue of $\mathscr{M}$. Another characterisation of λ to belong to the discrete spectrum is through the *eigenprojection*

$$P_\lambda := \frac{1}{2i\pi}\int_{\Gamma_\lambda}(z-\mathscr{M})^{-1}\,\mathrm{d}z\,, \tag{18.47}$$

where Γ_λ is a contour that enlaces only λ as an element of the spectrum. $P_\lambda : \mathsf{H} \to \mathsf{Dom}(\mathscr{M}) \subset \mathsf{H}$ is a bounded operator which commutes with $\mathscr{M}$ and does not depend on the choice of the contour Γ_λ. We say that λ has *finite algebraic multiplicity* when the range of P_λ is finite-dimensional. In this case, λ is a discrete eigenvalue of $\mathscr{M}$. Moreover, the range of P_λ coincides with the algebraic eigenspace of λ. It is an invariant subspace of $\mathscr{M}$ of finite dimension and such that the spectrum of $\mathscr{M}_{|\mathsf{R}(P_\lambda)}$ equals $\{\lambda\}$.

Finally, we recall three standard results. For the proofs see [13, Chap. I.3], [13, Thm. IX.2.1] and [18, Thm. XVII.2.1], respectively.

Lemma 18.6. *Let* $(\mathscr{M}, \mathsf{Dom}(\mathscr{M}))$ *be a closed operator in a Hilbert space* H. *Let us equip* $\mathsf{Dom}(\mathscr{M})$ *with the graph norm* $\|\cdot\|_{\mathscr{M}}$, *which makes* $(\mathsf{Dom}(\mathscr{M}), \|\cdot\|_{\mathscr{M}})$ *a new Hilbert space. Let* $\mathcal{M}$ *be the operator* $\mathscr{M}$ *reconsidered as an operator from* $(\mathsf{Dom}(\mathscr{M}), \|\cdot\|_{\mathscr{M}})$ *to* H. *The following properties hold:*

(i) $\mathcal{M}$ *is bounded,*

(ii) $\mathcal{M}$ *is Fredholm if and only if* $\mathscr{M}$ *is Fredholm.*
In this case, $\mathrm{ind}(\mathcal{M}) = \mathrm{ind}(\mathscr{M})$.

Lemma 18.7. *Let* $(\mathscr{M}, \mathsf{Dom}(\mathscr{M}))$ *be a closed invertible operator and consider another operator* $(\mathscr{P}, \mathsf{Dom}(\mathscr{M}))$ *in a common Hilbert space* H. *Assume that* $(\mathscr{M} + \mathscr{P}, \mathsf{Dom}(\mathscr{M}))$ *is closed and* $\mathscr{P}\mathscr{M}^{-1}$ *is compact. Then the operator* $(\mathscr{M} + \mathscr{P}, \mathsf{Dom}(\mathscr{M}))$ *is Fredholm and* $\mathrm{ind}(\mathscr{M} + \mathscr{P}) = \mathrm{ind}(\mathscr{M}) = 0$.

Lemma 18.8. *Let* $(\mathscr{M}, \mathsf{Dom}(\mathscr{M}))$ *be a closed operator in a Hilbert space* H *with a non-empty resolvent set and let* $\triangle$ *be an open connected subset of*

$$\{z \in \mathbb{C} \ : \ \mathscr{M} - z \quad \textit{is Fredholm}\}.$$

If $\triangle \cap \rho(\mathscr{M}) \neq \emptyset$, *then* $\mathsf{sp}(\mathscr{M}) \cap \triangle$ *is a countable set, with no accumulation point in* $\triangle$, *consisting of eigenvalues of* $\mathscr{M}$ *with finite algebraic multiplicities.*

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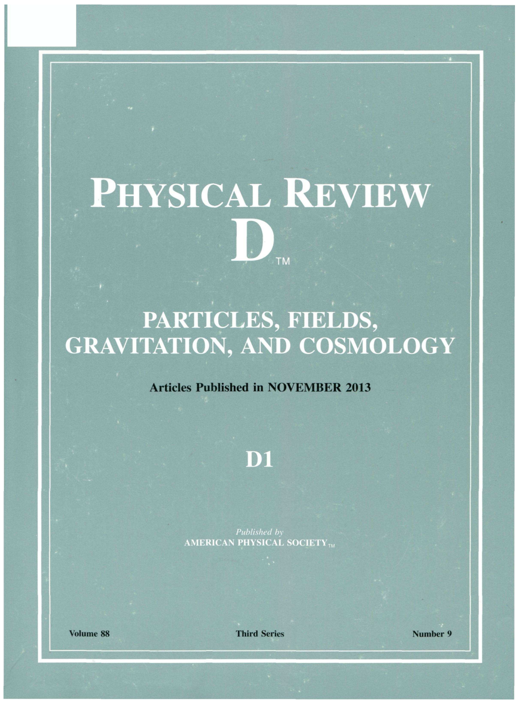
Part III

Pseudospectra

Chapter 19

On the metric operator for the imaginary cubic oscillator



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On the metric operator for the imaginary cubic oscillator

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Abstract. We show that the eigenvectors of the $\mathcal{PT}$-symmetric imaginary cubic oscillator are complete, but do not form a Riesz basis. This results in the existence of a bounded metric operator having intrinsic singularity reflected in the inevitable unboundedness of the inverse. Moreover, the existence of non-trivial pseudospectrum is observed. In other words, there is no quantum-mechanical Hamiltonian associated with it via bounded and boundedly invertible similarity transformations. These results open new directions in physical interpretation of $\mathcal{PT}$-symmetric models with intrinsically singular metric, since their properties are essentially different with respect to self-adjoint Hamiltonians, for instance, due to spectral instabilities.

19.1 Introduction

At the turn of the millennium, Bender *et al.* came up with the idea to extend quantum mechanics by considering Hamiltonians that are invariant under a space-time reflection $\mathcal{PT}$ rather than being Hermitian [1, 2]. The development of the so-called $\mathcal{PT}$-*symmetric quantum mechanics* was in fact initiated in these papers by considering a prominent Hamiltonian

$$H = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + ix^3. \tag{19.1}$$

While this operator is manifestly non-Hermitian, it is invariant under a simultaneous space reflection $\mathcal{P}$ ($x \mapsto -x$) and time reversal $\mathcal{T}$ (complex conjugation). Moreover, numerical studies suggested that the spectrum of H is *real*, which was later proved in [3, 4]. The Hamiltonian (19.1) can be considered as a prototype of many other examples of $\mathcal{PT}$-symmetric Hamiltonians that have been so far studied in a still growing literature (see [5, 6] and references therein). $\mathcal{PT}$-symmetric models found applications in various domains of physics – namely in optics [7, 8, 9, 10, 11], solid state [12], Bose-Einstein condensates [13], LRC circuits [14, 15], superconductivity [16, 17], electromagnetism [18, 19], and reflectionless scattering [20].

It is commonly accepted that a *quantum-mechanical* interpretation of $\mathcal{PT}$-symmetry must be implemented through a similarity transformation Ω, *i.e.*

$$h := \Omega H \Omega^{-1}, \tag{19.2}$$

where h is a self-adjoint operator, *i.e.* $h = h^\dagger$. This intertwining relation is closely related to the *quasi-Hermiticity* [21, 22]

$$\Theta H = H^\dagger \Theta, \tag{19.3}$$

where Θ is a positive operator often called *metric operator* (its special variant $\mathcal{PC}$ was suggested in Refs. [2, 23]). Hamiltonian H with property (19.3) is called quasi-Hermitian because it is actually Hermitian with respect to the modified inner product $\langle \cdot, \Theta \cdot \rangle$. The relation between Ω and Θ is the decomposition of a positive operator $\Theta = \Omega^\dagger \Omega$. The essential idea is that a non-Hermitian H can be viewed as an alternative representation of a Hermitian operator h.

The advantage of the above described representation (19.2) stems from the observation that the Hermitian counterpart h for a differential albeit non-Hermitian operator H has typically a non-local and very complicated structure. This was demonstrated for a class of operators with non-Hermitian (not necessarily $\mathcal{PT}$-symmetric) point interactions in [25, 26, 27], where, in addition, explicit formulae for the similarity transformation Ω, metric operator Θ, $\mathcal{C}$ operator, and similar self-adjoint operator h were presented in a closed form. Nevertheless, the non-Hermiticity and non-locality are not always equivalent in the described sense [28, 29, 30].

Partly motivated by the relevance of the cubic interaction in quantum field theory, the problem of similarity of the Hamiltonian (19.1) to a self-adjoint operator was investigated in several works [23, 24, 31]. However, due to the complexity of the task, the approach used in these papers was necessarily formal, based on developing the metric into an infinite series composed of unbounded operators. There has been no proof of the quasi-Hermiticity of the imaginary cubic oscillator so far. The objective of the present note is to establish the following intrinsic facts about the metric of (19.1):

1. *There exists a bounded metric.* That is, operator (19.1) is quasi-Hermitian in the sense of (19.3) with bounded Θ.

2. *No bounded metric with bounded inverse exists.* That is, any metric operator for (19.1) necessarily possesses an inevitable singularity.

We have chosen the prominent Hamiltonian (19.1) to prove the negative result 2 just because the ix^3 potential is considered as the *fons et origo* of $\mathcal{PT}$-symmetric quantum mechanics [1, 2]. However, the absence of bounded or boundedly invertible metric is by far not restricted to the Hamiltonian (19.1) only. For instance, the method of the present note also applies to an equally extensively studied $x^2 + ix^3$ potential and many others, see Eq. (19.17) and the surrounding text.

Our results have important consequences for the physical interpretation of the $\mathcal{PT}$-symmetric Hamiltonians. If the metric happens to be singular (*i.e.* unbounded, not invertible or unboundedly invertible), the quantum-mechanical interpretation using the similarity transformation is lost. Indeed, the eigenvectors, despite possibly being complete, do not form a "good" basis, *i.e.* an unconditional (Riesz) basis. The spectrum of such highly non-self-adjoint operators does not contain sufficient information about the system and in addition to the reality and (algebraic) simplicity of the spectrum, more involved spectral-theoretic properties (such as basicity, pseudospectrum, *etc.*) must be taken into account.

Our result about the singularity of any metric may seem negative at the first glance. However, we believe that in the same way as the exceptional points represent one of the most interesting configurations, where important physical phenomena arise, the established intrinsic singularities in the metric operator are precisely the point where new developments of the physics of $\mathcal{PT}$-symmetric models may originate.

This paper is organized as follows. In Section 19.2 we emphasize some aspects of unbounded operators and defects of quasi-Hermiticity based on singular metrics. In Section 19.3 we recall known facts about the imaginary cubic oscillator and perform our proofs of the new properties regarding the metric operator. Finally, in Section 19.4 we refer to some open problems and comment on possible extensions of our results.

19.2 Infinite-dimensional subtleties

While the concepts of similarity to a self-adjoint operator and quasi-Hermiticity work smoothly if the dimension of the underlying Hilbert space is finite, *i.e.* for matrices, essential difficulties may appear in the infinite-dimensional spaces. The reason is obviously in the unboundedness of operators, which unavoidably restricts their domains of definitions to a non-trivial subset of the Hilbert space. Therefore, the sense in which equalities (19.2) and (19.3) hold must be carefully explained. We focus on the metric operator further, nonetheless, the similarity transformation may be discussed along the same lines.

Relation (19.3) is an operator equality and as such it requires that the operator domains $\mathsf{D}(\Theta H)$ and $\mathsf{D}(H^\dagger\Theta)$ are equal in addition to the validity of the corresponding vector identity $\Theta H\psi = H^\dagger\Theta\psi$ for every $\psi \in \mathsf{D}(\Theta H) \cap \mathsf{D}(H^\dagger\Theta)$. Problems arise if the involved operators are unbounded, since one of the operator domains of the products or their intersection might be reduced to a single element 0. To avoid such pathological situations, it is usually assumed that the metric operator Θ is bounded. Then the above requirements reduce to the mapping property $\Theta[\mathsf{D}(H^\dagger)] \subset \mathsf{D}(H)$ and the quasi-Hermitian identity should hold for every $\psi \in \mathsf{D}(H)$.

If, in addition to the boundedness, Θ is boundedly invertible, then some fundamental and extremely useful properties of self-adjoint operators are valid for H as well: real spectrum, spectral decomposition, spectral stability with respect to perturbations, unitary evolution (in a topologically equivalent Hilbert space), *etc.* However, if the metric becomes singular, none of the mentioned properties is guaranteed by the validity of (19.3). As a matter of fact, as we demonstrate in this paper, the imaginary cubic oscillator and many other $\mathcal{PT}$-symmetric Hamiltonians, despite possessing real spectra, exhibit pathological features with respect to self-adjoint behaviour, due to the intrinsic singularities of the metric (and therefore also in $\mathcal{C}$-operators and similarity transformations). Let us demonstrate the defects of theories with singular metrics in the following subsections.

19.2.1 Spectrum

Let $\mathcal{H}$ be a complex Hilbert space. The *spectrum* is meaningfully defined only for closed operators, *i.e.* those operators H for which the elements $\{\psi, H\psi\}$ with $\psi \in \mathsf{D}(H)$ form a closed linear subspace of $\mathcal{H} \times \mathcal{H}$. If $\mathcal{H}$ were finite-dimensional, then the spectrum of H, $\sigma(H)$, would be exhausted by eigenvalues, *i.e.* those complex numbers λ for which $H - \lambda$ is not injective. In general, however, there are additional parts of spectra composed by those λ which are not eigenvalues but $H - \lambda : \mathsf{D}(H) \to \mathcal{H}$ is not bijective: depending on whether the range $\mathsf{R}(H - \lambda)$ is dense in $\mathcal{H}$ or not, one speaks about the *continuous* or *residual* spectrum, respectively. In other words, the complement of the spectrum of H, called the *resolvent set* of H, $\rho(H)$, is composed of all the complex numbers z for which the resolvent operator $(H - z)^{-1} : \mathcal{H} \to \mathcal{H}$ exists and is bounded.

It is an important property of self-adjoint operators that their (total) spectrum is always non-empty, real and that the residual spectrum is empty. For non-self-adjoint operators, however, the spectrum can be empty or cover the whole complex plane, see *e.g.* [28, 32].

Let us demonstrate how singular metrics lead to pathological situations as regards spectral properties. Let H be an operator with purely discrete spectrum (*i.e.* just isolated eigenvalues with finite multiplicities) and assume that the similarity relation (19.2) holds with unbounded Ω^{-1}. Then $\mathsf{R}(h-\lambda) \subset \mathsf{R}(\Omega) \neq \mathcal{H}$ for every $\lambda \in \mathbb{C}$. Consequently, the whole complex plane except for the set of eigenvalues of H belongs to the continuous spectrum of h. Summing up, *the continuous spectrum is not preserved by unbounded similarity transformations.* It is a striking phenomenon since the continuous part of spectrum contains physical energies corresponding to scattering/propagating states.

A similar argument shows that unbounded Θ satisfying (19.3) with $\mathsf{D}(\Theta) \supset \mathsf{D}(H)$ and $\Theta[\mathsf{D}(H)] \subset \mathsf{D}(H^\dagger)$ cannot exist for closed operators H with a physically reasonable property $\sigma(H) \neq \mathbb{C}$. In this way, one can also show that the $\mathcal{C}$-operator of [33] for (19.1) cannot exist.

19.2.2 Eigenbasis

Eigenfunctions of self-adjoint operators corresponding to different eigenvalues are mutually orthogonal. Furthermore, the set of all eigenfunctions $\{\psi_n\}_{n=1}^\infty$ of a self-adjoint operator with purely discrete spectrum can be normalized in such a way that it forms a *complete orthonormal family* in the Hilbert space $\mathcal{H}$. Recall that the completeness means that the orthogonal complement in $\mathcal{H}$ of the linear span of the family consists only of the zero function only. A necessary and sufficient condition for completeness of an orthonormal family $\{\psi_n\}_{n=1}^\infty$ is the validity of the Parseval equality

$$\forall \psi \in \mathcal{H}, \qquad \sum_{n=1}^{\infty} |\langle \psi_n, \psi \rangle|^2 = \|\psi\|^2. \tag{19.4}$$

In this case we also have the unique expansion

$$\forall \psi \in \mathcal{H}, \qquad \psi = \sum_{n=1}^{\infty} c_n \psi_n. \tag{19.5}$$

That is, $\{\psi_n\}_{n=1}^\infty$ is a *basis* in $\mathcal{H}$.

Eigenfunctions of non-Hermitian operators are typically not orthogonal. Even worse, they may not form a basis or even not a complete family. In this respect, it is absolutely essential to stress that the completeness of a non-orthonormal family $\{\psi_n\}_{n=1}^\infty$ does not imply that any $\psi \in \mathcal{H}$ admits a unique expansion (19.5); see *e.g.* [34] for further details.

The notion of "eigenbasis" is so important in quantum mechanics that one needs to have a replacement for (19.4) in the case of eigenfunctions of non-Hermitian operators. This is provided by the notion of *Riesz basis*

$$\forall \psi \in \mathcal{H}, \qquad C^{-1}\|\psi\|^2 \le \sum_{n=1}^{\infty} |\langle \psi_n, \psi \rangle|^2 \le C\|\psi\|^2 \tag{19.6}$$

with a positive constant C independent of ψ. Eigenfunctions of an operator H with purely discrete spectrum form a Riesz basis if, and only if, H is quasi-Hermitian (19.3) with bounded and boundedly invertible metric Θ.

As in the case of spectrum, *Riesz-basicity property is not preserved by unbounded transformations.* As a matter of fact, it is the objective of the present paper to show that the eigenfunctions of (19.1) do not form a Riesz basis, so that the metric Θ is necessarily singular. Any claim of the type "(19.1) is similar to a self-adjoint operator" is thus necessarily of doubtful usefulness for physics, since H and h appearing in (19.2) would have very different basicity properties.

19.2.3 Pseudospectrum

The notion of pseudospectra arose as a result of the realization that several pathological properties of highly non-Hermitian operators were closely related. We refer to by now classical monographs by Trefethen and Embree [35] and Davies [34] for more information on the subject, physical and numerical applications, and many references.

Given a positive number ε, we define the *pseudospectrum* of H by

$$\sigma_\varepsilon(H) := \left\{ z \in \mathbb{C} \;\middle|\; \|(H-z)^{-1}\| > \varepsilon^{-1} \right\}, \tag{19.7}$$

with the convention that $\|(H-z)^{-1}\| = \infty$ for $z \in \sigma(H)$. The pseudospectrum always contains an ε-neighbourhood of the spectrum:

$$\left\{ z \in \mathbb{C} \;\middle|\; \operatorname{dist}\big(z, \sigma(H)\big) < \varepsilon \right\} \subset \sigma_\varepsilon(H)\,. \tag{19.8}$$

Since equality holds here if H is self-adjoint (or more generally normal), it follows that the notion of pseudospectra becomes trivial for such operators. On the other hand, if H is "highly non-self-adjoint", the pseudospectrum $\sigma_\varepsilon(H)$ is typically "much larger" than the ε-neighbourhood of the spectrum.

For non-Hermitian operators the pseudospectra are much more reliable objects than the spectrum itself. Probably the strongest support for this claim is due to phenomenon of *spectral instability*: very small perturbations may drastically change the spectrum of a non-Hermitian operator. For instance, new complex eigenvalues can appear very far from the original ones. On the other hand, perturbations whose norm is less than ε still lie inside $\sigma_\varepsilon(H)$. These effects were extensively studied in numerics, hydrodynamics, optics, *etc.* (see [35] and references therein).

Of course, such pathological situations do not occur for self-adjoint operators whose spectrum is changed at most by the norm of the perturbation. It is also impossible for operators similar to self-adjoint operators by bounded and boundedly invertible similarity transformations. On the other hand, *the pseudospectrum is not preserved by unbounded transformations* (we refer to [36] for a warning discussion of the shifted harmonic oscillator in this context). The pseudospectrum thus represents a useful test whether a given non-Hermitian operator can be similar to a self-adjoint one via a physically reasonable transformation. In this paper we show that the pseudospectrum of (19.1) is highly non-trivial.

19.2.4 Singular metric?

The observations made in previous subsections constitute a strong support for our belief that the singular metrics are not relevant objects for physical interpretation of non-Hermitian Hamiltonians, since they yield only singular similarity transformations. However, putting it differently, singular metrics necessarily lead to fundamentally new physics, since the transformed operators exhibit completely different properties.

In this context we feel necessary to mention that there exists a recent attempt of Mostafazadeh [37], reproducing equivalently the original idea of Kretschmer and Szymanowski [38], to include singular metric operators into the notion of quasi-Hermiticity. It involves a construction of a self-adjoint operator to which the original non-Hermitian operator with purely discrete real spectrum is similar "at any cost". Analogous ideas for unbounded $\mathcal{C}$-operators can be found in [39]. However, any such strategy has important drawbacks that cannot be avoided. The problem with singular metric is mentioned already in [22], where an example of operator possessing bounded metric operator without bounded inverse and having *non-real spectrum* was constructed. As a corollary, Diedonné states: *"in spite of the quasi-Hermiticity (without bounded inverse of* Θ*), there is for instance no hope of building functional calculus that would follow more or less the same pattern as the functional calculus of self-adjoint operators"*.

The drawbacks consist in that the aforementioned non-self-adjoint pathologies of H are completely ignored when analysing the "similar" self-adjoint operator h instead. This can be illustrated already for two-by-two matrices: a Jordan-block matrix H and a diagonal matrix h with the same real eigenvalues. Although the matrices possess the same (real) spectrum, their respective properties are very different, particularly the basicity properties of eigenvectors and spectral stability with respect to small perturbations. But the construction of [38, 37], when used in finite dimension, simply means that the authors disregard the Jordan-block structure of the non-Hermitian matrix H and associate to it just the diagonal matrix h with same eigenvalues. The metric operator and "similarity transformation" are non-invertible in this case. However, equality (19.3) and a weaker variant of (19.2), *i.e.* $\Omega H = h\Omega$, do hold. Stating that h should in any reasonable sense represent H is obviously very doubtful, since, for instance, all the physics of exceptional points would be omitted.

In infinite-dimensional spaces the situation is even more complex, since another possibility of singularity of metric exists, namely the unboundedness of the inverse. Although this may seem to be a minor issue or only a technical problem of infinite dimension, such an interpretation is very misleading. The pathological properties of non-self-adjoint H with only unboundedly invertible metric may be much more serious than existence of finite-dimensional Jordan blocks, *i.e.* usual exceptional points. In the latter case, although the metric cannot be invertible, the eigenvectors together with generalized ones may form a Riesz basis. In other words, except a finite-dimensional subspace, H is similar to a self-adjoint operator. Therefore a version of the spectral decomposition (generalized Jordan form) may be available and the spectrum of H may be stable with respect to small perturbations. This is not the case of the imaginary cubic oscillator, where there is no Riesz basis of eigenvectors and no spectral stability: complex eigenvalues may appear very far from the unperturbed real ones despite the norm of the perturbation is arbitrarily small.

19.3 Imaginary cubic oscillator

Let us begin by properly introducing the Hamiltonian (19.1) as a closed realization in the Hilbert space $L^2(\mathbb{R})$. We consider the *maximal realization* of the differential expression (19.1) by taking for the operator domain of H the maximal domain

$$\mathsf{D}(H) := \left\{\psi \in L^2(\mathbb{R}) \,|\, -\psi'' + ix^3\psi \in L^2(\mathbb{R})\right\}. \tag{19.9}$$

By an approach of [40, Sec. VII.2], based on a distributional Kato's inequality, it follows that such a defined operator H is *m-accretive* and that it coincides with the closure of (19.1) initially defined on infinitely smooth functions of compact support. (The difficulties with the existence of different closed extensions, *cf* [41, 42], do not arise here since, $\Re V$ is trivially bounded from below.)

Now it can be rigorously verified that H is $\mathcal{PT}$-*symmetric*, *i.e.* $[H, \mathcal{PT}] = 0$, where the commutator should be interpreted as $\mathcal{PT}H\psi = H\mathcal{PT}\psi$ for all $\psi \in \mathsf{D}(H)$, with $(\mathcal{P}\psi)(x) := \psi(-x)$ and $(\mathcal{T}\psi)(x) := \overline{\psi(x)}$. Moreover, since the adjoint $H^\dagger$ of H is simply obtained by taking $-i$ instead of i in the definition of the operator (including the operator domain), it can be also verified that H is $\mathcal{P}$-*self-adjoint*, $H^\dagger = \mathcal{P}H\mathcal{P}$, and $\mathcal{T}$-*self-adjoint*, $H^\dagger = \mathcal{T}H\mathcal{T}$. The latter is a particularly useful property for non-self-adjoint operators since it implies that the residual spectrum of H is empty [43].

As an immediate consequence of the fact that H is m-accretive, we know that the spectrum of H is located in the right complex half-plane. Furthermore, it has been shown in [3, 4] that *all eigenvalues of H are real* and simple (in the sense of geometric multiplicity). The algebraic simplicity has been established in [44, 45]. The fact that the *spectrum of H is purely discrete* follows from the compactness of its resolvent. The latter can be deduced from the identity

$$\mathsf{D}(H) = \left\{\psi \in H^2(\mathbb{R}) \,|\, x^3\psi \in L^2(\mathbb{R})\right\} \tag{19.10}$$

established in [46] and the compact embedding of this set into $L^2(\mathbb{R})$. Furthermore, the authors of [46] show that the resolvent of H is a Hilbert-Schmidt operator. The key ingredient in the proof is the explicit knowledge of the resolvent kernel of H^{-1} that can be written in terms of Hankel functions with known asymptotics. A deeper analysis of the resolvent of H reveals that it actually belongs to the trace class [47]; alternatively, one can use a general result of [48].

19.3.1 Completeness of eigenfunctions

Let us show that the eigenfunctions of H form a complete set in $L^2(\mathbb{R})$. Recall that the completeness of $\{\psi_n\}_{n=1}^\infty$ means that the span of ψ_n is dense in $L^2(\mathbb{R})$, or equivalently $\left(\mathrm{span}\{\psi_n\}_{n=1}^\infty\right)^\perp = \{0\}$. Nevertheless, we stress that the result on completeness does not imply that any ψ admits the unique expansion (19.5).

The m-accretivity of H implies $\Re\langle\psi, H\psi\rangle \geq 0$ for all $\psi \in \mathsf{D}(H)$. Consequently, $-iH$ is dissipative, *i.e.* $\Im\langle\psi, H\psi\rangle \leq 0$ for all $\psi \in \mathsf{D}(H)$. It is then easy to check that the imaginary part of the resolvent of $-iH$ at $\xi < 0$ is non-negative, *i.e.*,

$$\frac{1}{2i}\left((-iH - \xi)^{-1} - (iH^\dagger - \xi)^{-1}\right) \geq 0 \tag{19.11}$$

in the sense of forms. Since the resolvent is trace class, it is enough to apply the completeness theorem [49, Thm.VII.8.1] to the operator $(-iH - \xi)^{-1}$.

More specifically, it follows by this result that H has a complete system of eigenvectors and generalized eigenvectors. The latter, however, do not appear in our situation since all the eigenvalues are algebraically simple (see above).

19.3.2 Existence of a bounded metric

Already at this stage, we can show that there exists a bounded metric for H. We would like to emphasize that this follows actually in general from the reality and simplicity of eigenvalues and completeness of eigenfunctions for H. We remark that $H^\dagger$ shares these properties due to the simplicity of eigenvalues and $\mathcal{T}$- or $\mathcal{P}$-self-adjointness of H.

In detail, let H be a densely defined and closed operator such that $\rho(H) \cap \rho(H^\dagger) \cap \mathbb{R} \neq \emptyset$ and let z_0 be a number from this intersection. Then the existence of a bounded positive Θ satisfying (19.3) is equivalent to the fact that the resolvent of H satisfies (19.3), *i.e.*,

$$\Theta(H - z_0)^{-1} = (H^\dagger - z_0)^{-1}\Theta. \tag{19.12}$$

Thus we can transfer the problem of finding the metric for an unbounded H to the same problem for its bounded resolvent. Using [22, Prop.3], which is in fact the construction of a bounded metric using the well-known formula

$$\Theta := \sum_{n=1}^\infty c_n \phi_n \langle\phi_n, \cdot\rangle \tag{19.13}$$

with ϕ_n being the eigenfunctions of $H^\dagger$ and $c_n > 0$ tending to zero sufficiently fast, yields the following: If all the eigenvalues of $H^\dagger$ are real and the associated eigenfunctions ϕ_n are complete, then a bounded metric for $(H - z_0)^{-1}$, and therefore for H, exists.

In our situation, we know that all the eigenvalues of (19.1) as well as its adjoint are simple and real, for z_0 we can take any negative number due to m-accretivity of H and $H^\dagger$, and we have shown that the eigenfunctions of H and therefore also $H^\dagger$ are complete. Hence the existence of a bounded Θ follows.

19.3.3 Singularity of any metric

After the two preceding positive results, we show now that any metric for the imaginary cubic oscillator is singular, *i.e.* either unbounded or unboundedly invertible. We proceed by contradiction. Let there exist a bounded positive operator Θ with bounded inverse satisfying (19.3). Then the following norm estimate for the resolvent holds:

$$\left\|(H - z)^{-1}\right\| \leq \frac{C}{|\Im z|} \tag{19.14}$$

for every $z \in \mathbb{C}$ such that $\Im z \neq 0$, where C is a positive constant bounded by $\left\|\sqrt{\Theta}\right\|\left\|\sqrt{\Theta^{-1}}\right\|$. By establishing a lower bound to the resolvent appearing in (19.14), we show that the inequality (19.14) cannot hold. The lower bound follows by a direct construction of a continuous family of approximate eigenstates of complex energies far from the spectrum due to Davies [50].

Using the strategy in [50, Thm. 2], we consider $\|(H - \sigma z)^{-1}\|$ with $\sigma > 0$ large and $0 < \arg z < \pi/2$. By a simple scaling argument in x, the problem can be transferred into a semi-classical one, namely $\|(H - \sigma z)^{-1}\| = \sigma^{-1}\|(H_h - z)^{-1}\|$, where

$$H_h := -h^2 \frac{\mathrm{d}^2}{\mathrm{d}x^2} + ix^3, \tag{19.15}$$

with $h := \sigma^{-5/6}$. In order to apply [50, Thm. 1], we have to verify that $\Im V'(a) \neq 0$, where $V(x) := ix^3$ and a is obtained from the relation $z = \eta^2 + ia^3$ with $\eta \in \mathbb{R} \setminus \{0\}$. However, this can be easily checked for $\Im V'(a) = 3a^2$ and $a \neq 0$ since $\Im z \neq 0$ by assumption. It then follows from [50, Thm. 1] that the norm of the resolvent of H_h diverges faster than any power of h^{-1} as $h \to 0$. More specifically, there exists positive h_0 and for each $n > 0$ a positive constant c_n such that if $h \in (0, h_0)$ then

$$\left\|(H_h - z)^{-1}\right\| \geq \frac{c_n}{h^n}. \tag{19.16}$$

The relation between H and H_h provides an analogous claim for $\|(H - \sigma z)^{-1}\|$ and therefore the resolvent bound (19.14) when combined with (19.16) cannot hold if n is chosen sufficiently large (namely, $n > 6/5$).

19.4 Concluding remarks

Although the imaginary cubic oscillator (19.1) is $\mathcal{PT}$-symmetric with purely real and discrete spectrum, it cannot be similar (via a bounded and boundedly invertible transformation) to any self-adjoint operator or, equivalently, the eigenfunctions of H cannot form the Riesz basis. We remark that the question whether eigenvectors of H form a basis remains open.

We established the existence of a bounded metric, which is in fact equivalent to the completeness of eigenfunctions that we proved and the reality and simplicity of eigenvalues. However, the singular nature of any metric is inevitable. The latter was established by semiclassical tools, namely the pseudomode construction due to [50]. The method of proof implies that (19.1) possesses a very non-trivial pseudospectrum and regions of strong spectral instabilities, *cf* (19.7) and (19.16). In the language of exceptional points, the imaginary cubic oscillator possesses an “intrinsic exceptional point” that is much stronger than any exceptional point associated with finite Jordan blocks, *cf* subsections 19.2.4, 19.3.3.

The method of this paper, namely the disproval of quasi-Hermiticity with bounded and boundedly invertible metric based on the localized semiclassical pseudomodes, does not restrict to the particular Hamiltonian (19.1). It also applies to the already mentioned $x^2 + ix^3$ potential, and to many others. As a large class of admissible operators let us mention for instance the Schrödinger operators considered by Davies [50]:

$$-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \sum_{m=1}^{2n} c_m x^m, \tag{19.17}$$

where the constant c_{2n} has positive real and imaginary parts; then the corresponding closed realization is an m-sectorial operator. Later, the results of [50] were substantially generalized to higher dimensions and pseudodifferential operators in [51, 52].

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Chapter 20

Pseudospectra in non-Hermitian quantum mechanics

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Pseudospectra in non-Hermitian quantum mechanics

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Abstract. We propose giving the mathematical concept of the pseudospectrum a central role in quantum mechanics with non-Hermitian operators. We relate pseudospectral properties to quasi-Hermiticity, similarity to self-adjoint operators, and basis properties of eigenfunctions. The abstract results are illustrated by unexpected wild properties of operators familiar from $\mathcal{PT}$-symmetric quantum mechanics.

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20.1 Introduction

In the highly non-normal case, vivid though the image may be, the location of the eigenvalues may be as fragile an indicator of underlying character as the hair colour of a Hollywood actor.

Trefethen and Embree, [77, p. 11]

It has long been known to numerical analysts that many important spectral properties of self-adjoint operators are lost when considering non-normal operators. In the 2005 monograph [77], Trefethen and Embree discuss decades of ongoing research and advocate the use of pseudospectra instead of spectra when studying a matrix or operator which is non-self-adjoint or non-normal.

In this paper we stress the importance of pseudospectra, a set which measures the instability of the spectrum of a non-normal operator, in the so-called "non-Hermitian quantum mechanics". Contrary to a common misconception, we demonstrate that the spectrum alone contains by far insufficient information to draw any quantum-mechanically relevant conclusions for non-Hermitian operators. In particular, the fact that the spectrum of an operator is real, or even the presence of a reduction to a self-adjoint operator using an unbounded similarity transformation, is not sufficient to guarantee that an operator with non-trivial pseudospectrum has a meaning in the context of conventional quantum mechanics.

By non-Hermitian quantum mechanics we mean the attempts of Bender *et al.* [15, 16] to extend quantum mechanics to include observables represented by $\mathcal{PT}$-symmetric non-Hermitian operators, see [1], with real spectra. Here, $\mathcal{PT}$-symmetry refers to the invariance of an operator H on the Hilbert space $L^2(\mathbb{R}^d)$ with respect to a simultaneous parity and time reversal, *i.e.*,

$$[H, \mathcal{PT}] = 0\,, \tag{20.1}$$

where $(\mathcal{P}\psi)(x) := \psi(-x)$ and $(\mathcal{T}\psi)(x) := \overline{\psi(x)}$. It has been argued that if the operator possesses, in addition to the obvious $\mathcal{PT}$-symmetry, a special hidden symmetry – a so-called $\mathcal{C}$-symmetry – then indeed the spectrum of H is real. It has furthermore been suggested that a consistent quantum theory can be built by changing the inner product into one for which the operator H is Hermitian and the time evolution is unitary. The procedure can be understood by the concept of pseudo-Hermiticity as developed by Mostafazadeh [52, 53, 54]: a $\mathcal{CPT}$-symmetric operator can be transformed into a self-adjoint operator $H_{\mathrm{sa}} = H_{\mathrm{sa}}^*$ via a similarity transformation Ω, *i.e.*,

$$H_{\mathrm{sa}} = \Omega H \Omega^{-1}\,. \tag{20.2}$$

The latter is the basis for a possible quantum-mechanical interpretation of H as an equivalent representation of a physical observable which would be conventionally represented by the self-adjoint operator H_{sa}.

If Ω in (20.2) is bounded and boundedly invertible, *cf* [2], although not necessarily unitary, then indeed the spectra of H_{sa} and H coincide and the pseudospectra are related by simple approximate inclusions; see

(20.8). Moreover, if the spectrum is discrete, the eigenfunctions of H and $H_{\rm sa}$ share essential basis properties. In this case, the $\mathcal{PT}$-symmetry can be understood through an older notion of quasi-Hermiticity [30, 66] and the quantum-mechanical description of H via $H_{\rm sa}$ is consistent: H and $H_{\rm sa}$ represent the same physical system.

However, problems arise if Ω or Ω^{-1} entering the fundamental relation (20.2) are allowed to be unbounded. We list several potential pitfalls below. We do not claim that there are no physical problems where an unbounded similarity transformation could be useful (in fact, there are!), nevertheless, if any of the pathological situations described below occur, $H_{\rm sa}$ and H cannot be viewed as equivalent representatives of the same physical observable in quantum mechanics.

1. It is not always easy to give a good meaning to the operator identity (20.2) when taking into account the respective domains. The relation (20.2) may hold on some particular functions, *e.g.* $C_0^\infty(\mathbb{R}^d)$, but the operator identity may not be satisfied.

2. Spectra are not preserved by unbounded transformations. It may well happen that the spectrum of H is purely discrete, while $H_{\rm sa}$ has no eigenvalues or some continuous spectrum, and vice versa.

3. Unbounded transformations may turn a nice (even orthonormal) eigenbasis to a set of functions that cannot form any kind of reasonable basis.

4. Spectra of non-Hermitian operators are known to lie deep inside very large pseudospectra, while the pseudospectrum of a self-adjoint operator is just a tubular neighbourhood of its spectrum. Consequently, the spectrum of $H_{\rm sa}$ is stable under small perturbations, while an arbitrarily small perturbation of H can create eigenvalues very far from the spectrum of H.

5. Even if the spectrum of H were purely real, $-iH$ does not need to be the generator of a bounded semigroup. In fact, a wild behaviour of the pseudospectrum of H prevents to associate a bounded time-evolution to H via the Schrödinger equation (*cf* [26, Thm. 8.2.1]).

The objective of this paper is to demonstrate by a careful mathematical analysis that these commonly overlooked problems do appear in more or less famous models of non-Hermitian quantum mechanics and to emphasize that the concept of pseudospectra gives important information missing in prior works. In conclusion, the present study necessarily casts doubt on certain commonly accepted conclusions based on formal manipulations in the physical literature, *cf* the reviews [14, 55], particularly on the physical relevance of $\mathcal{PT}$-symmetry in the quantum-mechanical context. We notably refer to the concrete examples presented in Section 20.7 for specific controversies. We also remark that the unbounded time-evolution has been recently studied more explicitly for some of the models presented below, namely in [36] for the gauged oscillator (see Section 20.7.7) and in [8, 9] for quadratic operators (see Section 20.7.8).

Our approach relies on standard tools of modern functional analysis, nonetheless, several innovations appear. Particularly, we construct new pseudomodes for the (non-semiclassical) shifted harmonic oscillator, where the scaling leads to the fractional power of h, *cf* Theorem 20.2. We also give a new and very short proof of the rate of spectral projection growth for the rotated oscillator analysed previously in [27, 38, 79], *cf* Appendix 20.9. Last but not least, we establish an explicit unitary equivalence between the rotated and gauged oscillator (Swanson's model), which has not been noticed previously. We furthermore describe how to identify an equivalent rotated oscillator for each such quadratic operator in a class identified in [58].

The paper is organized as follows. In the Section 20.2 we summarize some basic properties of pseudospectra. Since $\mathcal{PT}$-symmetry is a special example of an antilinear symmetry, we briefly discuss pseudospectral properties of operators commuting with antiunitary operators in Section 20.3. Our main mathematical tool for proving the existence of large pseudospectra is stated as Theorem 20.1 of Section 20.4; it is based on a construction of pseudomodes of semiclassical operators adapted from [29]. In Section 20.5 we relate the pseudospectrum to the concept of quasi-Hermiticity and similarity to a self-adjoint operator. A relationship between basis properties of eigenfunctions is pointed out in Section 20.6. Finally, in Section 20.7 (which occupies the bulk of the paper), we present a number of non-self-adjoint ordinary differential operators exhibiting striking spectral and pseudospectral properties; they will serve as an illustration of the abstract operator-theoretic methods summarized in this paper. Certain technical proofs are reserved for the Appendix.

20.2 Pseudospectra

The notion of pseudospectra arose as a result of the realization that several pathological properties of highly non-Hermitian operators were closely related. We refer to by now classical monographs by Trefethen and Embree [77] and Davies [26] for more information on the subject and many references.

Let H be a closed densely defined operator (bounded or unbounded) on a complex Hilbert space $\mathcal{H}$. The *spectrum* of H, denoted by $\sigma(H)$, consists of those complex points z for which the resolvent $(H-z)^{-1}$ does not exist as a bounded operator on $\mathcal{H}$. If $\mathcal{H}$ were finite-dimensional, then the spectrum of H would be exhausted by eigenvalues (*i.e.* those complex numbers λ for which $H-\lambda$ is not injective). In general, however, there are additional parts of the spectrum composed of those λ which are not eigenvalues but for which $H-\lambda : \mathsf{D}(H) \to \mathcal{H}$ is not bijective: depending on whether the range $\mathsf{R}(H-\lambda)$ is dense in $\mathcal{H}$ or not, one speaks about the *continuous* or *residual* spectrum, respectively.

The complement of $\sigma(H)$ in $\mathbb{C}$ is called the *resolvent set* of H. The *numerical range* $\mathsf{Num}(H)$ of H is defined by the set of all complex numbers $(\psi, H\psi)$ where ψ ranges over all ψ from the operator domain $\mathsf{D}(H)$ with $\|\psi\| = 1$.

Given a positive number ε, we define the *ε-pseudospectrum* (or simply *pseudospectrum*) of H as

$$\sigma_\varepsilon(H) := \sigma(H) \cup \left\{ z \in \mathbb{C} \;\middle|\; \|(H-z)^{-1}\| > \varepsilon^{-1} \right\}; \tag{20.3}$$

sometimes the convention that $\|(H-z)^{-1}\| = \infty$ for $z \in \sigma(H)$ is used. (We refer to the interesting essays [67, 68] by Shargorodsky on the distinction between the definition of pseudospectra with strict and non-strict inequalities.) Here we summarize some basic well-known properties of pseudospectra.

• **Topology.** For every $\varepsilon > 0$, $\sigma_\varepsilon(H)$ is a non-empty open subset of $\mathbb{C}$ and any bounded connected component of $\sigma_\varepsilon(H)$ has a non-empty intersection with $\sigma(H)$. (If the spectrum of H is empty, then $\sigma_\varepsilon(H)$ is unbounded for every $\varepsilon > 0$.) These facts follow from the subharmonicity of $\|(H-z)^{-1}\|$ as a function of $z \notin \sigma(H)$ to $(0, \infty)$.

• **Relation to spectra.** The pseudospectrum always contains an ε-neighbourhood of the spectrum, and if $\mathbb{C} \setminus \overline{\mathsf{Num}(H)}$ is connected and has a non-empty intersection with the resolvent set of H, the pseudospectrum is in turn contained in an ε-neighbourhood of the numerical range:

$$\left\{ z \in \mathbb{C} \;\middle|\; \operatorname{dist}\big(z, \sigma(H)\big) < \varepsilon \right\} \subseteq \sigma_\varepsilon(H) \subseteq \left\{ z \in \mathbb{C} \;\middle|\; \operatorname{dist}\big(z, \overline{\mathsf{Num}(H)}\big) < \varepsilon \right\}. \tag{20.4}$$

The first inclusion follows from the bound $\|(H-z)^{-1}\| \geq \operatorname{dist}\big(z, \sigma(H)\big)^{-1}$, which is valid for any operator. Since equality holds there if H is self-adjoint (or more generally normal, *i.e.* $H^*H = HH^*$), it follows that the pseudospectra for such operators give no additional information not already given by the spectrum. On the other hand, if H is "highly non-self-adjoint", the pseudospectrum $\sigma_\varepsilon(H)$ is typically "much larger" than the ε-neighbourhood of the spectrum. In any case, the second inclusion shows that the pseudospectra are well behaved outside the numerical range.

• **Spectral instability.** There is an important property (known sometimes as the Roch-Silberman theorem [64], although the result is already mentioned in [63]) relating the pseudospectra to the stability of the spectrum under small perturbations:

$$\sigma_\varepsilon(H) = \bigcup_{\|V\| < \varepsilon} \sigma(H+V). \tag{20.5}$$

The importance of this property is summarized by the following statement from [25]:

> *Very large pseudospectra are always associated with eigenvalues which are very unstable with respect to perturbations. This is clearly of great importance to numerical analysts: if a spectral problem is unstable enough, no numerical procedure can enable one to find the eigenvalues, whose significance therefore becomes a moot point.*

The relation (20.5) likely lends the strongest support for the usage of pseudospectra instead of spectra in the case of non-Hermitian operators.

• **Pseudomodes.** A complex number z belongs to $\sigma_\varepsilon(H)$ if, and only if, $z \in \sigma(H)$ or z is a *pseudoeigenvalue* (or *approximate eigenvalue*), *i.e.*,

$$\|(H-z)\psi\| < \varepsilon \|\psi\| \quad \text{for some} \quad \psi \in \mathsf{D}(H). \tag{20.6}$$

Any ψ satisfying (20.6) is called a *pseudoeigenvector* (or *pseudoeigenfunction* or *pseudomode*). Again, for operators H which are far from self-adjoint, pseudoeigenvalues may not be close to the spectrum of H. This is particularly striking if we realize that these pseudoeigenvalues can be turned into true eigenvalues by a very small perturbation, *cf* (20.5). What is more, we can often construct very nice (*e.g.* smooth and with compact support) pseudoeigenfunctions; see Section 20.4 and the references therein.

• **Adjoints.** Using the identity $\|(H^* - \bar{z})^{-1}\| = \|(H-z)^{-1}\|$, it is easy to see that the pseudospectrum of H^* is given by the mirror image of $\sigma_\varepsilon(H)$ with respect to the real axis, *i.e.*,

$$\lambda \in \sigma_\varepsilon(H) \iff \overline{\lambda} \in \sigma_\varepsilon(H^*)\,. \tag{20.7}$$

• **Similarity.** Let the similarity relation (20.2) hold with a bounded and boundedly invertible operator Ω. Then the operators H and H_{sa} have the same spectra, but their pseudospectra may be very different, unless the *condition number* $\kappa := \|\Omega\|\|\Omega^{-1}\| \geq 1$ is fairly close to one. Indeed, we have

$$\sigma_{\varepsilon/\kappa}(H) \subseteq \sigma_\varepsilon(H_{\mathrm{sa}}) \subseteq \sigma_{\varepsilon\kappa}(H)\,. \tag{20.8}$$

20.3 Antilinear symmetry

We understand $\mathcal{PT}$-symmetry as a special example of invariance of a closed densely defined operator H with respect to an *antiunitary* transformation $\mathcal{S}$, *i.e.*,

$$[H, \mathcal{S}] = 0\,. \tag{20.9}$$

Recall that $\mathcal{S}$ is an antiunitary transformation if $\mathcal{S}$ is a bijective antilinear operator on $\mathcal{H}$ satisfying $(\mathcal{S}\phi, \mathcal{S}\psi) = (\psi, \phi)$ for every $\phi, \psi \in \mathcal{H}$. As usual for the commutativity of an unbounded operator and a bounded operator [44, Sec. III.5.6], we understand (20.9) by the operator relation $\mathcal{S}H \subseteq H\mathcal{S}$. In other words, whenever $\psi \in \mathsf{D}(H)$, the image $\mathcal{S}\psi$ also belongs to $\mathsf{D}(H)$ and $\mathcal{S}H\psi = H\mathcal{S}\psi$.

• **Symmetry.** It is well known that the spectra of $\mathcal{PT}$-symmetric operators on $L^2(\mathbb{R}^d)$ are symmetric with respect to the real axis. In our general situation (20.9), this follows from the identity

$$(H-z)^{-1} = \mathcal{S}^{-1}(H-\bar{z})^{-1}\mathcal{S}, \tag{20.10}$$

which is valid for any z in the resolvent set of H; the symmetry can then be deduced from (20.9). Furthermore, (20.10) yields the same relation for the pseudospectra of $\mathcal{S}$-symmetric operators H:

$$\lambda \in \sigma_\varepsilon(H) \iff \overline{\lambda} \in \sigma_\varepsilon(H)\,. \tag{20.11}$$

This identity holds trivially when the resolvent set of H is empty.

• **$\mathcal{J}$-self-adjointness.** An alternative framework for $\mathcal{PT}$-symmetric operators was suggested in [19] in terms of $\mathcal{J}$-self-adjoint operators. Here $\mathcal{J}$ is a *conjugation*, *i.e.* an antiunitary involution, and H is said $\mathcal{J}$*-self-adjoint* if $H^* = \mathcal{J}H\mathcal{J}$, *cf* [33, Sec. III.5]. (The present $\mathcal{J}$-self-adjointness should not be confused with a terminologically similar but different concept in Krein spaces [7, 37].) An example of such a $\mathcal{J}$ on $L^2(\mathbb{R}^d)$ is $\mathcal{T}$, *i.e.* complex conjugation. A particularly useful property of $\mathcal{J}$-self-adjoint operators is that their residual spectrum is always empty, *cf* [19].

20.4 Microlocal analysis

It was Davies [23] who first realized that and how semiclassical methods can be applied to the study of pseudospectra of non-Hermitian Schrödinger operators. Shortly thereafter, Zworski [81] pointed out that Davies' discoveries could be related to long-established results in the microlocal theory of partial differential operators due to Hörmander and others. We refer to a paper of Dencker, Sjöstrand and Zworski [29] for an important development of the idea in the context of pseudodifferential operators. We state here a version of their general result for the special case of differential operators with analytic coefficients in one dimension, in a formulation given in [77, Thm. 11.1].

We recall some standard notions first. Let $h > 0$ be a (small) parameter. Given continuous functions $a_j : \mathbb{R} \to \mathbb{C}$, with $j = 0, \dots, n$, we define a *symbol*

$$f(x,\xi) := \sum_{j=0}^{n} a_j(x)(-i\xi)^j\,, \qquad (x,\xi) \in \mathbb{R}^2\,, \tag{20.12}$$

and the associated *semiclassical differential operator*

$$H_h := \sum_{j=0}^{n} a_j(x)\, h^j\, \frac{\mathrm{d}^j}{\mathrm{d}x^j}\,, \qquad \mathsf{D}(H_h) := C_0^\infty(\mathbb{R})\,. \tag{20.13}$$

The *Poisson bracket* $\{\cdot,\cdot\}$ is defined as

$$\{u,v\} := \frac{\partial u}{\partial \xi}\frac{\partial v}{\partial x} - \frac{\partial u}{\partial x}\frac{\partial v}{\partial \xi} \tag{20.14}$$

and, for $u = f$, $v = \bar{f}$, it simplifies to

$$\{f,\bar{f}\} = 2i\left(\frac{\partial \Im f}{\partial \xi}\frac{\partial \Re f}{\partial x} - \frac{\partial \Re f}{\partial \xi}\frac{\partial \Im f}{\partial x}\right).$$

The closure of the set

$$\Lambda := \left\{f(x,\xi) \,:\, (x,\xi)\in\mathbb{R}^2,\ \frac{1}{2i}\{f,\bar{f}\}(x,\xi) > 0\right\} \tag{20.15}$$

is referred to as the *semiclassical pseudospectrum* of H_h, *cf* [29]. In the special case of H_h being a Schrödinger operator with an analytic potential, the condition $\frac{1}{2i}\{f,\bar{f}\}(x,\xi) > 0$ reduces to $\Im V'(x) \neq 0$ and $\xi \neq 0$, because the sign of ξ can be chosen freely, and it is also equivalent to the *twist condition* of [77, Sec. III.11]. The nonvanishing of $\{f,\bar{f}\}$ is a classical analogue of the operator H_h not being normal [29].

Theorem 20.1 (Semiclassical pseudomodes.)**.** *Let the functions a_j, $j = 0,\dots,n$, be analytic and let H_h be the semiclassical differential operator* (20.13)*. Then for any $z \in \Lambda$, there exist $C = C(z) > 1$, $h_0 = h_0(z) > 0$ and an h-dependent family of $C_0^\infty(\mathbb{R})$ functions $\{\psi_h\}_{0<h\le h_0}$ with the property that, for all $0 < h \le h_0$,*

$$\|(H_h - z)\psi_h\| < C^{-1/h}\,\|\psi_h\|.$$

Such of family of functions is called a pseudoeigenfunction (or *pseudomode*) for the operator H_h corresponding to *pseudoeigenvalue* (or *approximate eigenvalue*) z.

In Appendix 20.8, we include a proof of the theorem in the special case of Schrödinger operators.

The theorem can be generalized significantly beyond the restrictive assumption that the coefficients are globally analytic. As stated in [77, Thm. 11.1], one only needs that the a_j are analytic in a neighborhood of some $x_0 \in \mathbb{R}$ corresponding to an $(x_0,\xi_0) \in \mathbb{R}^2$ putting $z \in \Lambda$. Furthermore, [29] shows the existence of pseudomodes for pseudodifferential operators (which include differential operators) whose symbols are only assumed to be smooth (and bounded). The price of abandoning the assumption of analytic coefficients is a slower rate of growth. In the smooth case, instead of an upper bound of $C^{-1/h}\|\psi_h\|$ one has an upper bound for each $N \in \mathbb{N}$ and constant $C(N) > 0$ depending on N:

$$\|(H_h - z)\psi_h\| < \frac{h^N}{C(N)}\,\|\psi_h\|\,,$$

for all $0 < h \le h_0$. For the examples to follow, it will be sufficient to consider the analytic case as written in Theorem 20.1.

Although Theorem 20.1 is stated for semiclassical operators, scaling techniques allow its application to non-semiclassical operators where the spectral parameter tends to infinity. This is based on the principle that the semiclassical limit is equivalent to the high-energy limit after a change of variables; this principle is made concrete in many of the examples below. For further details, the reader could consult [82].

20.5 Metric operators

The similarity relation (20.2) is closely related to the *quasi-Hermiticity* of H:

$$H^*\Theta = \Theta H\,, \tag{20.16}$$

where Θ is a positive operator called a *metric* [30, 66]. The terminology comes from the observation that H is formally self-adjoint with respect to the modified inner product $\langle\cdot,\Theta\cdot\rangle$. More precisely, we have

Proposition 20.1. *The operator H is similar to a self-adjoint operator via a bounded and boundedly invertible positive transformation (*i.e. (20.2) *holds) if, and only if, H is quasi-Hermitian with a positive, bounded, and boundedly invertible metric (*i.e. (20.16) *holds).*

Proof. If H satisfies (20.16) with a bounded and boundedly invertible $\Theta > 0$, then the similarity relation (20.2) to a self-adjoint operator h holds with any Ω satisfying the decomposition $\Theta = \Omega^*\Omega$. Conversely, if (20.2) holds with a bounded and boundedly invertible Ω, then it is easy to check that (20.16) holds with $\Theta = \Omega^*\Omega > 0$. $\square$

As emphasized in [71], fundamental problems arise if one starts to relax the conditions on boundedness or bounded invertibility of the transformations.

• **Trivial pseudospectra.** We say that the pseudospectrum of H is *trivial* if there exists a fixed constant C such that, for all $\varepsilon > 0$,

$$\sigma_\varepsilon(H) \subseteq \{z \in \mathbb{C} \mid \operatorname{dist}(z, \sigma(H)) < C\varepsilon\} .$$

That is, the pseudospectrum of H is contained in a tubular neighbourhood of the spectrum of H (although of possibly larger radius than ε). Recalling the text below (20.4), the pseudospectra of self-adjoint and normal operators are trivial.

Proposition 20.2. *Let H be quasi-Hermitian* (20.16) *with a positive, bounded and boundedly invertible metric. Then the pseudospectrum of H is trivial.*

Proof. It is enough to recall Proposition 20.1 and (20.8); the condition number plays the role of the constant C. □

Proposition 20.2 can be conveniently used in the reverse sense, where the presence of nontrivial pseudospectrum for a given operator H immediately implies that the operator cannot possess a physically relevant (*i.e.* bounded and boundedly invertible) metric.

20.6 Basis properties

Let H be an operator with compact resolvent throughout this section. Then the spectrum of H consists entirely of isolated eigenvalues with finite (algebraic) multiplicities. Below, we recall that similarity to a self-adjoint operator, or quasi-Hermiticity, is equivalent to having the set of eigenvectors form a Riesz basis.

First, we recall the definition of a basis. We say that $\{\psi_k\}_{k=1}^\infty$ is a *(Schauder or conditional) basis* if every $\psi \in \mathcal{H}$ has a unique expansion in the vectors $\{\psi_k\}$, *i.e.*

$$\forall \psi \in \mathcal{H}, \quad \exists! \{\alpha_k\}_{k=1}^\infty, \quad \psi = \sum_{k=1}^\infty \alpha_k \psi_k \, , \tag{20.17}$$

where the infinite sum is understood as a limit in the strong topology of $\mathcal{H}$.

• **Riesz basis.** We say that $\{\psi_k\}_{k=1}^\infty$, normalized to 1 in $\mathcal{H}$, forms a *Riesz (or unconditional) basis* if it forms a basis and the inequality

$$\forall \psi \in \mathcal{H}, \qquad C^{-1}\|\psi\|^2 \leq \sum_{k=1}^\infty |\langle \psi_k, \psi \rangle|^2 \leq C\|\psi\|^2 \tag{20.18}$$

holds with a positive constant C independent of ψ (see [26, Thm.3.4.5] for equivalent formulations). In view of the Parseval equality, for any self-adjoint operator with a purely discrete spectrum one may choose orthonormal eigenvectors which form a Riesz basis with $C = 1$. For non-self-adjoint operators, however, it is not even clear that the eigenfunctions form a basis or even a complete set in $\mathcal{H}$.

Proposition 20.3. *Let H be an operator with compact resolvent for which $\sigma(H) \subset \mathbb{R}$. Then H is quasi-Hermitian with a positive, bounded and boundedly invertible metric (*i.e. (20.16) *holds) if, and only if, the eigenfunctions of H form a Riesz basis (*i.e. (20.18) *holds).*

Proof. If H is quasi-Hermitian with bounded, boundedly invertible, and positive metric Θ, then, by Proposition 20.1, H is similar to a self-adjoint operator h via a bounded and boundedly invertible transformation Ω. Consequently, $\Omega\psi_k/\|\Omega\psi_k\|$ form a complete orthonormal family in $\mathcal{H}$ satisfying the Parseval inequality, from which (20.18) follows. Conversely, assuming (20.18), we construct a bounded and boundedly invertible positive operator $L := \sum_{k=1}^\infty \psi_k \langle \psi_k, \cdot \rangle$. It is easy to check that (20.16) holds with $\Theta = L^{-1}$. □

Combining Proposition 20.3 with Proposition 20.2, we see that the pseudospectrum can be employed as a useful indicator of whether a non-self-adjoint operator possesses a Riesz basis.

• **No basis.** Eigensystems of non-self-adjoint operators can have very wild basis properties. We recall that if $\{\psi_k\}_{k=1}^\infty$ is a basis, then there exists a sequence $\{\phi_k\}_{k=1}^\infty$ for which the pair $\{\psi_k\}, \{\phi_k\}$ is biorthogonal, *i.e.* $\langle \phi_m, \psi_n \rangle = \delta_{m,n}$, such that $\alpha_k = \langle \phi_k, \psi \rangle$, *cf* [26, Lem. 3.3.1]. Let us denote the associated one-dimensional projections as

$$P_k := \psi_k \langle \phi_k, \cdot \rangle. \tag{20.19}$$

The uniform boundedness principle is used to derive the following standard result.

Proposition 20.4. *If $\{\psi_k\}_{k=1}^\infty$ is a basis, then both P_k and $\sum_{k=1}^N P_k$ are uniformly bounded in $\mathcal{H}$.*

Proof. The definition (20.17) implies that, for every $\psi \in \mathcal{H}$,

$$\forall \varepsilon > 0,\ \exists N_{\psi,\varepsilon},\ \forall n, m > N_{\psi,\varepsilon}, \qquad \left\| \sum_{k=1}^{n} P_k\psi - \sum_{k=1}^{m} P_k\psi \right\| < \varepsilon\,. \tag{20.20}$$

In particular, putting $m := n-1$ and $\varepsilon := 1$, we obtain $\|P_n\psi\| < 1$ if $n > N_{\psi,\varepsilon}$. Consequently, $\sup_k \|P_k\psi\| < \infty$ for every $\psi \in \mathcal{H}$. Finally, the uniform boundedness principle [61, Thm. III.9] yields $\sup_k \|P_k\| < \infty$. The proof of the second claim is analogous, see also [26, Lem. 3.3.3]. □

For operators H with positive discrete spectrum, the basis property of the eigensystem of H may be excluded by the following corollary of [24, Thm. 3].

Proposition 20.5. *Let H be an operator with compact resolvent, let its eigenvalues be simple and satisfy $\lambda_n \geq bn^\beta$ for some $b, \beta > 0$ and all $n \in \mathbb{N}$ and let the corresponding eigenvectors form a basis. Then there exist positive constants k, m such that*

$$\|(H-z)^{-1}\| \leq k\frac{(1+|z|^2)^{\frac{m}{2}}}{|\Im z|}\,, \qquad z \notin \mathbb{R}. \tag{20.21}$$

In Section 20.7 we shall give a number of examples of non-self-adjoint operators which have no basis of (generalized) eigenvectors. This will immediately follow upon demonstrating that the norms of their eigenprojectors diverge or that the pseudospectrum of H does not obey the restriction (20.21). The resolution of the identity, which plays a central role in quantum mechanics, is simply not available.

• **Completeness.** There exist weaker notions of basis in the literature (*e.g.* Abel-Lidskii basis), but they are not nearly as useful in applications. The weakest is to merely require the *completeness* of $\{\psi_k\}_{k=1}^\infty$, *i.e.* that the span of $\{\psi_k\}_{k=1}^\infty$ is dense in $\mathcal{H}$, or equivalently $\big(\operatorname{span}\{\psi_k\}_{k=1}^\infty\big)^\perp = \{0\}$. We have a converse of Proposition 20.4 for a minimal complete set $\{\psi_k\}_{k=1}^\infty$, which implies that the projections P_k in (20.19) may be defined: if the sums of projectors $\sum_{k=1}^N P_k$ are uniformly bounded, then $\{\psi_k\}_{k=1}^\infty$ is a basis, *cf* [26, Lem. 3.3.3].

20.7 Examples

In this last section we present a number of examples exhibiting remarkable pseudospectral behaviour due to non-Hermiticity and use them to demonstrate that the concept of pseudospectrum is a more relevant consideration for the description of the operators, specifically in the context of quantum mechanics.

We restrict ourselves mainly to the concrete situation of one-dimensional differential operators familiar from "non-Hermitian quantum mechanics". However, we emphasize that there exist versions of Theorem 20.1 for partial differential (even pseudodifferential) operators too (see [81, 29]) and it is straightforward to construct similar examples with non-trivial pseudospectra in higher dimensions. Non-Hermitian spectral effects for $\mathcal{PT}$-symmetric waveguides were previously observed in [19, 49, 20].

To avoid complicated notation, we study an operator H which changes in each subsection. Where there is a parameter dependence, we may write a subscript as in H_h. The notation H_{sa} will denote a self-adjoint operator, related to H usually via a formal (unbounded) conjugation. The symbol C (occasionally with a subscript) will denote a generic constant which may change from line to line.

20.7.1 The imaginary Airy operator

The non-self-adjoint operator

$$H := -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + ix \qquad \text{on} \qquad L^2(\mathbb{R}) \tag{20.22}$$

arises in the Ginzburg-Landau model of superconductivity [10, 12, 11] and also in the study of resonances of quantum Hamiltonians with electric field via the method of complex scaling [40]. It is well defined as a closed operator when considered on its maximal domain

$$\mathsf{D}(H) := \left\{\psi \in L^2(\mathbb{R}) \mid -\psi'' + ix\psi \in L^2(\mathbb{R})\right\}. \tag{20.23}$$

Indeed, such a definition coincides with the closure of (20.22) initially defined on smooth functions of compact support, *cf* [33, Cor. VII.2.7]. More importantly, H is m-accretive, *i.e.*, the numerical range $\mathsf{Num}(H)$ is contained in the closed right complex half-plane and the resolvent bound $\|(H-z)^{-1}\| \leq |\Re z|^{-1}$ holds for all z with $\Re z < 0$. The adjoint H^* of H is simply obtained by replacing i with $-i$ in (20.22) and (20.23). Furthermore, H is $\mathcal{PT}$-symmetric and $\mathcal{T}$-self-adjoint.

• **Spectrum.** Integrating by parts, we easily check that

$$\begin{aligned}\|\psi'\|^2 &= \langle\psi',\psi'\rangle = \langle\psi,-\psi''\rangle \le \|\psi\|\|\psi''\| \le \delta\|\psi''\|^2+\delta^{-1}\|\psi\|^2\,, \qquad (20.24)\\ \|H\psi\|^2 &= \|\psi''\|^2+\|x\psi\|^2+2\Re\langle ix\psi,-\psi''\rangle = \|\psi''\|^2+\|x\psi\|^2+2\Re\langle i\psi,\psi'\rangle\\ &\ge \|\psi''\|^2+\|x\psi\|^2-2\|\psi\|\|\psi'\| \ge \|\psi''\|^2+\|x\psi\|^2-\delta\|\psi'\|^2-\delta^{-1}\|\psi\|^2\,,\end{aligned}$$

for every $\psi\in C_0^\infty(\mathbb{R})$ and $\delta>0$. Combining these inequalities for $\delta>0$ sufficiently small and using the density of $C_0^\infty(\mathbb{R})$ in $\mathsf{D}(H)$, we arrive at the non-trivial fact that

$$\mathsf{D}(H)=\left\{\psi\in W^{2,2}(\mathbb{R})\mid x\psi\in L^2(\mathbb{R})\right\}.$$

Here $W^{2,2}(\mathbb{R})$ denotes the usual Sobolev space of functions in $L^2(\mathbb{R})$ whose weak first and second derivatives belong to $L^2(\mathbb{R})$, *cf* [3]. Now it is clear that $\mathsf{D}(H)$ is compactly embedded in $L^2(\mathbb{R})$ and H is an operator with compact resolvent, *cf* [62, Thm. XIII.65]. It follows that the spectrum of H may consist of isolated eigenvalues only. However, the eigenvalue equation $H\psi=\lambda\psi$ implies that for any $c\in\mathbb{R}$ we also have $H\psi_c=\lambda_c\psi_c$ with $\psi_c(x):=\psi(x+c)$ and $\lambda_c:=\lambda-ic$. Consequently, the spectrum of H is empty,

$$\sigma(H)=\varnothing\,.$$

This is a peculiar property, possible for non-self-adjoint operators only. We deduce that H is not similar to a self-adjoint operator, via a bounded and boundedly invertible similarity transform.

• **Pseudospectrum.** While H has no spectrum, the pseudospectrum of H is far from trivial. *A priori*, we only know that the pseudospectrum is symmetric with respect to the real axis, *i.e.* (20.11) holds, which follows from the $\mathcal{PT}$-symmetry of H. In order to apply Theorem 20.1, we have to convert H into a semiclassical operator. This can be achieved by introducing the unitary transform $\mathcal{U}$ on $L^2(\mathbb{R})$ defined by

$$(\mathcal{U}\psi)(x):=\tau^{1/2}\psi(\tau x)\,, \qquad (20.25)$$

where $\tau\in\mathbb{R}$ is positive (and typically large in the sequel). Then

$$\mathcal{U}H\mathcal{U}^{-1}=\tau H_h \qquad\text{with}\qquad H_h:=-h^2\frac{\mathrm{d}^2}{\mathrm{d}x^2}+ix \qquad\text{and}\qquad h:=\tau^{-3/2}\,.$$

For the symbol $f=\xi^2+ix$ associated with H_h we have $\{f,\bar f\}=-4i\xi$. Hence, the interior of the semiclassical pseudospectrum is $\Lambda=\{z\in\mathbb{C}\mid\Re z>0\}$, using definition (20.15).

The same translation argument which shows that the spectrum is empty shows that

$$\|(H-z)^{-1}\|=\|(H-\Re z)^{-1}\|.$$

Note that $1\in\Lambda$. Applying the unitary relation and Theorem 20.1, there exists some $C>1$ where, for h sufficiently small (that is, $\tau>C_1$ for some $C_1>0$ sufficiently large),

$$\|(H-\tau)^{-1}\|=\tau^{-1}\|(H_h-1)^{-1}\|>h^{2/3}C^{1/h}\,.$$

We then have that $\tau\in\sigma_\varepsilon(H)$ whenever $\tau^{-1}C^{\tau^{3/2}}>\varepsilon^{-1}$. We may simplify the inequality by taking logarithms: it reads

$$\tau^{3/2}-\frac{\log\tau}{\log C}>\frac{1}{\log C}\log\frac{1}{\varepsilon}.$$

Since $\log\tau$ is negligible compared with $\tau^{3/2}$ for $\tau>0$ large, a sufficient condition to guarantee that $\tau\in\sigma_\varepsilon(H)$ is given by

$$\tau>C_2\left(\log\frac{1}{\varepsilon}\right)^{2/3}$$

with some $C_2>0$; this gives the correct order of growth as $\varepsilon\to 0$.

Since the resolvent norm only depends on the real part of the spectral parameter z, we arrive at the conclusion that there exist $C_1,C_2>0$ such that, for all $\varepsilon>0$,

$$\sigma_\varepsilon(H)\supseteq\left\{z\;\middle|\;\Re z\ge C_1\ \&\ \Re z\ge C_2\left(\log\frac{1}{\varepsilon}\right)^{2/3}\right\}.$$

In particular, for any ε there are complex points with positive real part and magnitude only logarithmically large in $1/\varepsilon$ that lie in the pseudospectrum $\sigma_\varepsilon(H)$.

A quite precise study of the resolvent norm of H as $\Re z\to\infty$ can be found in [18, Cor. 1.4].

• **Time evolution.** Since H is m-accretive, it is a generator of a one-parameter contraction semigroup, e^{-tH}, on $L^2(\mathbb{R})$. Here t can be interpreted as time, viewing $\psi(t,x) = e^{-tH}\psi(0,x)$ as arising as a solution of the parabolic equation $\partial_t\psi + H\psi = 0$. Using the Fourier transform, it is possible to show (*cf* [26, Ex. 9.1.7]) that

$$\|e^{-tH}\| = e^{-t^3/12}\,.$$

Note that the time decay rate is not determined by the (nonexistent) spectrum of H. In fact, the superexponential decay rate implies by itself that the spectrum of H must be empty. We refer to [12] for pseudospectral estimates on the decay of the semigroup in analogous higher-dimensional models.

20.7.2 The imaginary cubic oscillator

The non-self-adjoint (but $\mathcal{T}$-self-adjoint) operator

$$H := -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + ix^3 \qquad \text{on} \qquad L^2(\mathbb{R}) \tag{20.26}$$

is considered the *fons et origo* of $\mathcal{PT}$-symmetric quantum mechanics [15, 16], but it was also considered previously in the context of statistical physics and quantum field theory [34]. The existence of a metric operator and other spectral and pseudospectral properties of H have been recently analysed in [71]. Let us recall the basic results here, referring to the last article for more details and references.

• **Spectrum.** The operator H is again m-accretive when considered on its maximal domain (*i.e.* (20.23) with x replaced by x^3) and its resolvent is compact. Contrary to the imaginary Airy operator, the spectrum is not empty; it is composed of an infinite sequence of discrete real eigenvalues, *cf* [69, 32, 35]. As a new result, it is proved in [71] that the eigenfunctions form a complete set in $L^2(\mathbb{R})$.

• **Pseudospectrum.** Employing the unitary transform (20.25), we introduce a semiclassical analogue of H,

$$\mathcal{U}H\mathcal{U}^{-1} = \tau^3 H_h \qquad \text{with} \qquad H_h := -h^2\frac{\mathrm{d}^2}{\mathrm{d}x^2} + ix^3 \qquad \text{and} \qquad h := \tau^{-5/2}\,.$$

For the symbol f associated with H_h we now have $\{f,\bar{f}\} = -12i\xi x^2$, so that the interior of the semiclassical pseudospectrum is $\Lambda = \{z \in \mathbb{C} \mid \Re z > 0 \ \&\ \Im z \neq 0\}$.

The translation argument used for the imaginary Airy operator is unavailable for the imaginary cubic oscillator, but we nonetheless have by Theorem 20.1 for any $z \in \Lambda$, there exists $C > 0$ sufficiently large and h_0 sufficiently small that, for all $0 < h \leq h_0$,

$$\|(H - \tau^3 z)^{-1}\| = \tau^{-3}\|(H_h - z)^{-1}\| > h^{6/5} C^{1/h}\,. \tag{20.27}$$

One may check that the exponential growth in Theorem 20.1 may be made uniform on compact subsets $K \subset \Lambda$, as explained at the end of Appendix 20.8. What is more, one may extend the reasoning to include real $z > 0$, despite the fact that formally $z \notin \Lambda$: one only needs to verify (20.87) by hand, which is straightforward.

Since we are using a scaling argument, we may reduce to fixing $\delta > 0$ and letting

$$K = \{z \in \mathbb{C} \mid |z| = 1 \ \&\ |\arg z| < \pi/2 - \delta\}.$$

We therefore have that, for some positive constant C depending on δ, the pseudospectrum $\sigma_\varepsilon(H)$ contains $\tau^3 K$ so long as $\tau > 0$ is large enough to verify $\tau^{-3}C^{\tau^{5/2}} > \varepsilon^{-1}$. We may then identify τ^3 with the absolute value of the spectral parameter, and so $h = \tau^{-5/2} = |z|^{-5/6}$. Taking logarithms and discarding the negligible term involving logarithms, as before, allows us to conclude that, for any $\delta > 0$, there exist $C_1, C_2 > 0$ such that, for all $\varepsilon > 0$,

$$\sigma_\varepsilon(H) \supseteq \left\{ z \in \mathbb{C} \;\middle|\; |z| \geq C_1 \ \&\ |\arg z| < \left(\frac{\pi}{2} - \delta\right) \ \&\ |z| \geq C_2 \left(\log\frac{1}{\varepsilon}\right)^{6/5} \right\}. \tag{20.28}$$

Again, for any ε there are complex points with positive real part, non-zero imaginary part, and large magnitude that lie in the pseudospectrum $\sigma_\varepsilon(H)$. A numerical computation of some pseudospectral lines of H is presented in Figure 20.1. The asymptotic behaviour of the pseudospectral lines is studied in [18, Prop. 4.1]. The result is surprising because it implies the existence of pseudoeigenvalues very far from the spectrum of H. In view of (20.5), it follows that a very small perturbation V added to H can create (genuine) eigenvalues very far from the spectrum of the unperturbed operator H. In this way, the spectrum is highly unstable.

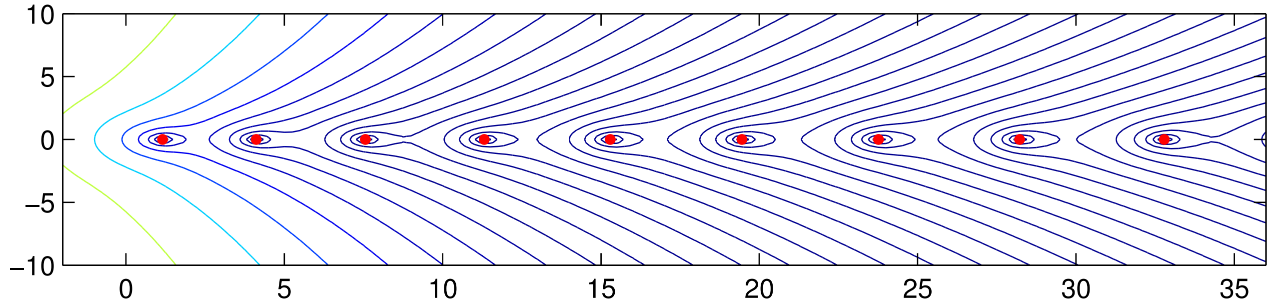

Figure 20.1: Spectrum (red dots) and pseudospectra (enclosed by the blue contour lines) of the imaginary cubic oscillator.

As a consequence of the existence of the highly non-trivial pseudospectrum, we also get that H is not quasi-Hermitian with a bounded and boundedly invertible metric (Proposition 20.2), it is not similar to a self-adjoint operator via bounded and boundedly invertible transformations (Proposition 20.1), and the eigenfunctions of H do not form a Riesz basis (Proposition 20.3). It has been shown recently in [39] that the norms of the spectral projections grow as

$$\lim_{k\to\infty} \frac{\log \|P_k\|}{k} = \frac{\pi}{\sqrt{3}}, \tag{20.29}$$

and therefore the eigenfunctions cannot form a basis, *cf* Proposition 20.4. Alternatively, we can derive the latter using Proposition 20.5 and (20.27).

20.7.3 An advection-diffusion operator

The examples which follow are similar to self-adjoint operators via *unbounded* transformations. In order to emphasize the danger of formal manipulations when the transformations are allowed to be unbounded, in this subsection we present a very simple non-self-adjoint operator for which heuristic approaches would lead to a number of striking paradoxes. The example is borrowed from [60, 25], although it is natural to expect that it has appeared in many other works. We are indebted to E. B. Davies and M. Marletta [28] for telling us about this example and for proposing the possibility of the non-invariance of point spectra discussed below.

Consider the differential operator

$$H := -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{\mathrm{d}}{\mathrm{d}x} \qquad \text{on} \qquad L^2(\mathbb{R})\,. \tag{20.30}$$

The diffusion term $-\mathrm{d}^2/\mathrm{d}x^2$ corresponds to the familiar free Hamiltonian in quantum mechanics, which is self-adjoint when defined on $W^{2,2}(\mathbb{R})$. The advection term represents a relatively bounded perturbation with relative bound equal to zero, so that $\mathsf{D}(H) = W^{2,2}(\mathbb{R})$, *cf* [44, Sec. IV.1.1]. Employing the first line of (20.24), we find

$$|\Im(\psi, H\psi)| \le \|\psi\|\|\psi'\| = \|\psi\|\sqrt{\Re(\psi, H\psi)}$$

for every $\psi \in \mathsf{D}(H)$. It follows that the numerical range $\mathsf{Num}(H)$ is contained in the parabolic domain $\Sigma := \{z \in \mathbb{C} \mid \Re z \ge 0 \;\&\; |\Im z|^2 \le \Re z\}$. In particular, H is not only m-accretive but even m-sectorial, meaning that, in addition, its numerical range is a subset of a sector in the complex plane. By conjugating with the Fourier transform, it is easy to check that the spectrum of H coincides with the parabola

$$\sigma(H) = \partial\Sigma = \{z \in \mathbb{C} \mid \Re z \ge 0 \;\&\; |\Im z|^2 = \Re z\}\,,$$

see Figure 20.2.

• **Non-invariance of the continuous spectrum.** Completing the square, we may write

$$H = -\left(\frac{\mathrm{d}}{\mathrm{d}x} - \frac{1}{2}\right)^2 + \frac{1}{4}\,.$$

This suggests that the similarity transformation $\Omega := e^{-x/2}$ *formally* maps H to a shifted free Hamiltonian

$$H_{\mathrm{sa}} := -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{1}{4}\,, \tag{20.31}$$

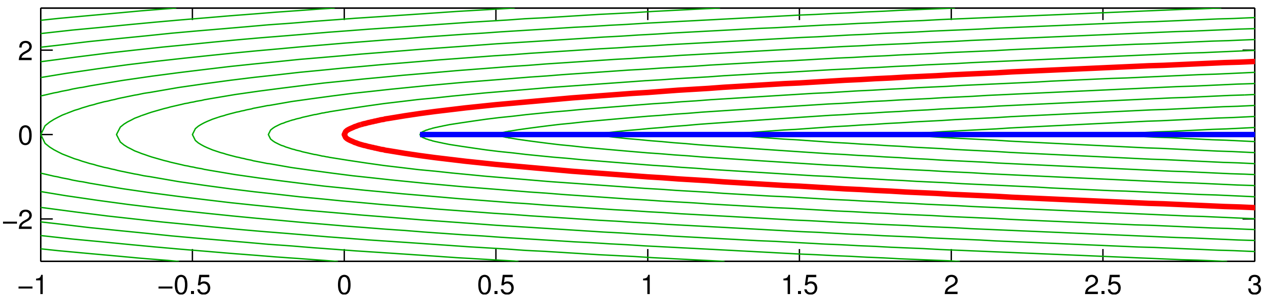

Figure 20.2: Spectrum of the advection-diffusion operator (red parabola) compared with the spectrum of the shifted free Hamiltonian (blue line) to which the former is formally similar and pseudospectral contours (green curves parallel to the parabola).

which is self-adjoint on $\mathsf{D}(H_{\mathrm{sa}}) := W^{2,2}(\mathbb{R})$. The word "formally" is absolutely essential here, since neither Ω nor Ω^{-1} is bounded and (20.2) cannot hold as an operator identity. Nevertheless, one can check that (20.2) holds on smooth functions with compact support, which form a dense subset of both $\mathsf{D}(H)$ and $\mathsf{D}(H_{\mathrm{sa}})$. Now we arrive at a surprising paradox because

$$\sigma(H_{\mathrm{sa}}) = [\tfrac{1}{4}, \infty)$$

substantially differs from the complex parabolic spectrum of H, see Figure 20.2. This is caused by the fact that the continuous spectrum is in general not preserved by unbounded similarity transformations.

• **Non-invariance of the point spectrum.** The situation is in fact even worse, since it may also happen that even the eigenvalues are not preserved by the similarity transformation Ω. Let us perturb the self-adjoint Hamiltonian H_0 by a smooth non-trivial potential $V \leq 0$ which has a compact support in $\mathbb{R}$. Then it is well known (see, *e.g.*, [65, Cor. 4.5.2]) that the self-adjoint operator $H_{\mathrm{sa}} + V$ possesses at least one eigenvalue $\lambda < 1/4$. The corresponding eigenfunction ψ has asymptotics $\exp(-\sqrt{1/4-\lambda}\,|x|)$ as $x \to \pm\infty$. It is also known that λ is positive provided that the supremum norm of V is sufficiently small, *cf* [72]. However, the corresponding "eigenfunction" $\Omega^{-1}\psi$ of $H + V$ is not admissible because it is not square-integrable on $\mathbb{R}$.

• **Pseudospectrum.** Even if H is not self-adjoint (nor $\mathcal{T}$-self-adjoint or $\mathcal{PT}$-symmetric), it is normal (and in fact real). Hence the pseudospectra are trivial; see Figure 20.2. The situation would be very different if we considered (20.30) on a finite interval $(0, L)$, subject to Dirichlet boundary conditions. Let us denote this operator by $H^{(L)}$. Then the similarity transformation $\Omega = e^{-x/2}$ is bounded and boundedly invertible and (20.2) with the self-adjoint operator $H_{\mathrm{sa}}^{(L)}$ that acts as (20.31) on $(0, L)$, subject to Dirichlet boundary conditions, is well defined. We indeed have

$$\sigma(H^{(L)}) = \sigma(H_{\mathrm{sa}}^{(L)}) = \left\{ \left(\frac{\pi k}{L}\right)^2 + \frac{1}{4} \;\middle|\; k = 1, 2, \dots \right\}.$$

However, the pseudospectra of $H^{(L)}$ substantially differ from those of $H_{\mathrm{sa}}^{(L)}$; the former approach the parabola $\partial\Sigma$ in the limit as $L \to \infty$, thus reflecting better the wild spectral instability of the limit; see Figure 20.2. We refer to [60] for more details.

20.7.4 The rotated harmonic oscillator

The quantum Hamiltonian of the harmonic oscillator

$$H_{\mathrm{sa}} := -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + x^2 \qquad \text{on} \qquad L^2(\mathbb{R}) \tag{20.32}$$

is self-adjoint on its maximal domain. The operator H_{sa} has compact resolvent and its eigenvalues are well-known:

$$\sigma(H_{\mathrm{sa}}) = \{2k+1 \mid k = 0, 1, \dots\}. \tag{20.33}$$

Of course, the pseudospectrum of H_{sa} is trivial; see Figure 20.4.

• **Creation and annihilation operators.** Recall also the factorization $H_{\rm sa} = a^*a + 1$, where a^* and a are the creation and annihilation operators defined by

$$a^* := -\frac{\mathrm{d}}{\mathrm{d}x} + x\,, \qquad a := \frac{\mathrm{d}}{\mathrm{d}x} + x\,, \tag{20.34}$$

with $\mathsf{D}(a) = \mathsf{D}(a^*) := W^{1,2}(\mathbb{R}) \cap L^2(\mathbb{R}, x^2\,\mathrm{d}x)$. As the notation suggests, a^* and a are mutually adjoint. The operator domain $\mathsf{D}(a)$ in fact coincides with the form domain of $H_{\rm sa}$, for which $C_0^\infty(\mathbb{R})$ is a core. We incidentally remark that a^* and a represent interesting examples of highly non-self-adjoint operators for which the resolvent operator is not defined at any point of the complex plane:

$$\sigma(a^*) = \sigma(a) = \mathbb{C}\,.$$

Indeed, $\psi(x) := \exp(\lambda x - x^2/2)$ is an eigenfunction of a for every $\lambda \in \mathbb{C}$. On the other hand, the point spectrum of a^* is empty, but every complex point belongs to the residual spectrum of a^*. The latter follows by the general fact that the orthogonal complement of the range of a densely defined closed operator in a Hilbert space is equal to the kernel of its adjoint.

• **Complex dilation.** The rotated harmonic oscillator H is *formally* obtained by the similarity transformation (20.2), where Ω^{-1} is the complex dilation operator defined by $(\Omega^{-1}\psi)(x) := e^{i\theta/4}\psi(e^{i\theta/2}x)$. If θ were purely imaginary, Ω^{-1} would be unitary, but we assume $\theta \in \mathbb{R}$ when Ω^{-1} is in fact unbounded. The formal computation yields

$$H = -e^{-i\theta}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + e^{i\theta}x^2 = e^{-i\theta}\left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + e^{2i\theta}x^2\right) \qquad \text{on} \qquad L^2(\mathbb{R})\,, \tag{20.35}$$

which we take as a definition and restrict to $|\theta| < \pi/2$. The operator H is sometimes referred to as Davies' oscillator due to his important investigation [22] (see also [26, Sec. 14.5] for a summary and other references). The presence of the prefactor $e^{-i\theta}$ in our definition is inessential, but it is useful for symmetry reasons. In particular, we have

$$|\Im(\psi, H\psi)| \leq |\tan\theta|\; \Re(\psi, H\psi) = |\sin\theta|\; (\psi, H_{\rm sa}\psi)$$

for every $\psi \in C_0^\infty(\mathbb{R})$. That is, under our restriction on θ, the operator H can be understood as obtained as a relatively form bounded perturbation of $H_{\rm sa}$, keeping the same form domain $\mathsf{D}(a)$. The numerical range $\mathsf{Num}(H)$ lies in the symmetric sector $\{z \in \mathbb{C} \mid |\Im z| \leq |\tan\theta| \Re z \;\&\; \Re z \geq 0\}$. Unless $\theta = 0$, H is neither self-adjoint nor $\mathcal{PT}$-symmetric, but it is always $\mathcal{T}$-self-adjoint.

• **Spectrum and pseudospectrum.** The resolvent of H is again compact and the spectrum coincides with that of $H_{\rm sa}$:

$$\sigma(H) = \sigma(H_{\rm sa})\,. \tag{20.36}$$

In particular, the spectrum is real. However, the pseudospectrum and basis properties of the eigenfunctions are very different from the self-adjoint situation. In the same way as we applied Theorem 20.1 to the imaginary Airy operator or cubic oscillator, we find

$$\Lambda = \{z \in \mathbb{C}\backslash\{0\} \mid |\arg z| < \theta\}.$$

When $\theta = 0$, Λ is empty and $H_{\rm sa}$ is self-adjoint, so that we know that its pseudospectrum is trivial. If $\theta \neq 0$, however, we have exponential growth for the resolvent indicated by Theorem 20.1, which may be made uniform for a compact subset contained in the interior of the semiclassical pseudospectrum. What is more, from [41, Thm. 1.1, Rem. 1.3], we have upper bounds for the resolvent norm of essentially the same exponential type, though the gap in the constant leaves much to be understood about the precise behaviour.

A scaling argument similar to that used for (20.28) gives us an idea of size of the ε-pseudospectrum, which includes more or less those $z \in \mathsf{Num}(H)$ for which $|z| > C\log(1/\varepsilon)$, which grows very slowly as $\varepsilon \to 0$.

Specifically, for any $\delta > 0$, we have from Theorem 20.1 that there exist $C_1, C_2 > 0$ such that, for all $\varepsilon > 0$,

$$\sigma_\varepsilon(H) \supseteq \left\{ z \;\middle|\; |z| > C_1 \;\&\; |\arg z| \leq \theta - \delta \;\&\; |z| > C_2 \log\frac{1}{\varepsilon} \right\}.$$

The numerical range inequality (20.4) gives that

$$\sigma_\varepsilon(H) \subseteq \{z \mid \mathrm{dist}(z, \mathsf{Num}(H)) < \varepsilon\}\,.$$

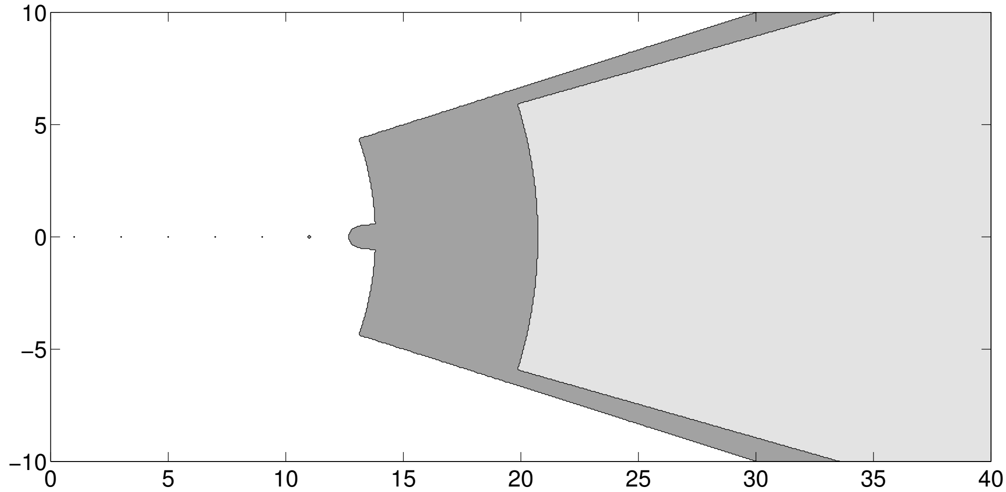

Figure 20.3: Diagram of region (dark gray) which contains $\sigma_\varepsilon(H)$ and region with pseudomodes (light gray) which is definitely contained in $\sigma_\varepsilon(H)$.

What is more, rescaling the upper bound [41, Eq. (1-8)] gives that there exists $C_3 > 0$ for which

$$\left\|(H-z)^{-1}\right\| \leq \frac{C_3 e^{C_3|z|}}{\operatorname{dist}(z,\sigma(H))}.$$

We therefore see that z cannot be in the pseudospectrum unless it is logarithmically large in $1/\varepsilon$ or close to the spectrum:

$$\sigma_\varepsilon(H) \subseteq \left\{ z \;\middle|\; |z| > \frac{1}{C_3}\left(\log\frac{1}{\varepsilon} - \log C_3\right)\right\} \cup \left\{ z \;\middle|\; \operatorname{dist}(z,\sigma(H)) < C_3\varepsilon e^{C_3|z|}\right\}.$$

In Figure 20.3, we have a diagram illustrating the sorts of regions containing and contained by the pseudospectrum. We emphasize that the constants involved were chosen by hand and do not reflect a precise application of the relevant theorems. As in the previous examples, for any $\varepsilon > 0$ there are complex points with positive real part, non-zero imaginary part, and large magnitude that lie in the pseudospectrum $\sigma_\varepsilon(H)$; see Figure 20.4. The asymptotic behaviour of the pseudospectrum has been also studied in [56, 18].

• **Wild basis properties.** H_0 is self-adjoint and we know *a priori* that its eigenfunctions (after normalization) form a complete orthonormal family in $L^2(\mathbb{R})$. If $\theta \neq 0$, it is still true that the eigenfunctions of H and H^* (after a suitable normalization) form a biorthonormal sequence. However, the eigenfunctions do not form a Riesz basis or even a basis, as can be deduced from the non-trivial pseudospectrum (*cf* Propositions 20.3 and 20.5).

Furthermore, it was shown in [27] that the norms of the spectral projections of H associated with eigenvalues $2k+1$ grow exponentially as $k \to \infty$, and the exact exponential rate of growth was identified. This exponential growth rate was sharpened in [38, Thm. 1.2, Rem. 1.3] to include an asymptotic expansion for the remainder and a generalization to operators including $-\mathrm{d}^2/\mathrm{d}x^2 + e^{2i\theta}|x|^{2m}$ for $m \in \mathbb{N}$ and natural restrictions on θ.

In the case of the rotated harmonic oscillator, one has from [79, Cor. 1.7, Ex. 3.6] an exact integral formula leading to a similar asymptotic expansion and a simplification of the formula for the exponential growth rate to

$$\lim_{k\to+\infty} \frac{\log\|P_k\|}{k} = \frac{1}{2}\log\left(\frac{1+|\sin\theta|}{1-|\sin\theta|}\right). \tag{20.37}$$

The new and very short proof of this formula using special functions is given in Appendix 20.9.

Summing up, despite the reality of the spectrum of H and the existence of a formal similarity transformation given by a complex dilation, we see that H exhibits very different properties from those enjoyed by self-adjoint operators.

20.7.5 The shifted harmonic oscillator

The shift operator T_t is, for $t \in \mathbb{R}$, well defined as a bounded operator on $L^2(\mathbb{R})$ by the formula $(T_t\psi)(x) := \psi(x+t)$. It is in fact a unitary group $T_t = e^{t\,\mathrm{d}/\mathrm{d}x}$ with the self-adjoint generator $-i\,\mathrm{d}/\mathrm{d}x$ defined on $W^{1,2}(\mathbb{R})$ being the familiar momentum operator in quantum mechanics. Let $H_{\rm sa}$ be again the self-adjoint harmonic oscillator (20.32) and perform the *formal* conjugation (20.2) with the *unbounded* operator $\Omega := T_{-i}$. Then we arrive at the non-self-adjoint operator

$$H = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + (x+i)^2 \qquad \text{on} \qquad L^2(\mathbb{R}), \tag{20.38}$$

which we again take as a definition. The extra term $2ix - 1$ clearly represents a relatively bounded perturbation of H_{sa} with the relative bound equal to zero, so that $\mathsf{D}(H) = \mathsf{D}(H_{\mathrm{sa}})$. It is also relatively form bounded with relative bound equal to zero, so that H is m-sectorial on $\mathsf{D}(a)$. The operator H is $\mathcal{PT}$-symmetric and $\mathcal{T}$-self-adjoint.

• **Spectrum and pseudospectrum.** The above remarks on the smallness of the perturbations imply that the resolvent of H is compact. Notice that conjugation with the Fourier transform casts H into a unitarily equivalent operator

$$\hat{H} := \left(-i\frac{\mathrm{d}}{\mathrm{d}x} - i\right)^2 + x^2,$$

which is related to (20.32) via the unbounded similarity transform $\hat{\Omega}\psi(x) := e^x\psi(x)$. Using that the eigenfunctions of the harmonic oscillator (20.32) are known to decay superexponentially, it can be showed that

$$\sigma(H) = \sigma(H_{\mathrm{sa}}),$$

analogously to (20.36).

Numerical computations show that the pseudospectrum of H is non-trivial; see Figure 20.4. Because of the different scaling properties of x^2 and x, Theorem 20.1 is not directly applicable. Nonetheless, we show, by adapting the construction of pseudomodes, that there are indeed large complex pseudoeigenvalues in parabolic regions of the complex plane.

Theorem 20.2. *Let H be the operator from* (20.38). *Fix $\varepsilon > 0$. Then there exists $C > 0$ sufficiently large such that for all $z \in \mathbb{C}$ for which $\Re z > C$ and*

$$|\Im z| \le 2(1-\varepsilon)\sqrt{\Re z},$$

we have the resolvent lower bound

$$\|(H - z)^{-1}\| \ge \frac{1}{C} e^{\sqrt{\Re z}/C}.$$

We postpone the proof to Appendix 20.8.

• **Wild basis properties.** The pseudospectral criteria of Propositions 20.2, 20.3 and 20.5 show that the eigenfunctions of H cannot form a Riesz basis or even a basis. Moreover, explicit formulas for the eigenfunctions can be used to prove their completeness in $L^2(\mathbb{R})$ and to find the rate of the norms of spectral projections, namely

$$\lim_{k\to+\infty} \frac{\log\|P_k\|}{\sqrt{k}} = 2^{3/2}, \tag{20.39}$$

see [51, Sec. 2] for the detailed proof.

20.7.6 The decaying and singular potential perturbations of harmonic oscillator

Examples in previous sections show that the perturbations of harmonic oscillator may have very non-trivial pseudospectra and wild basis properties, although the spectrum is preserved. In order not to leave an impression that this is typical for any perturbation of the harmonic oscillator, we mention that the system of all generalized eigenfunctions of perturbations $H = H_{\mathrm{sa}} + V$ of H_{sa} in (20.32) contains a Riesz basis when the perturbation V is multiplication by a function satisfying, for instance, $V \in L^p(\mathbb{R}), 1 \le p < \infty$, or V is a finite linear combination of δ-potentials with complex couplings; *cf* [4, 5, 50] for details and additional examples. It is also showed in these works that the eigenvalues of the perturbed operator H, excluding possibly a finite number, remain simple. Therefore, if the perturbation satisfies some symmetries, *e.g.* it is $\mathcal{PT}$-symmetric, we can conclude that the eigenvalues of H are real, again up to a finite number. Moreover, if we insert a sufficiently small coupling constant ε in front of V, we obtain that all eigenvalues are simple and real. When the coupling constant is increased, low lying eigenvalues may collide, create a Jordan block, and then become complex. This behaviour is illustrated in Figure 20.5 for an example of H where V is $\mathcal{PT}$-symmetric and has the form (20.40).

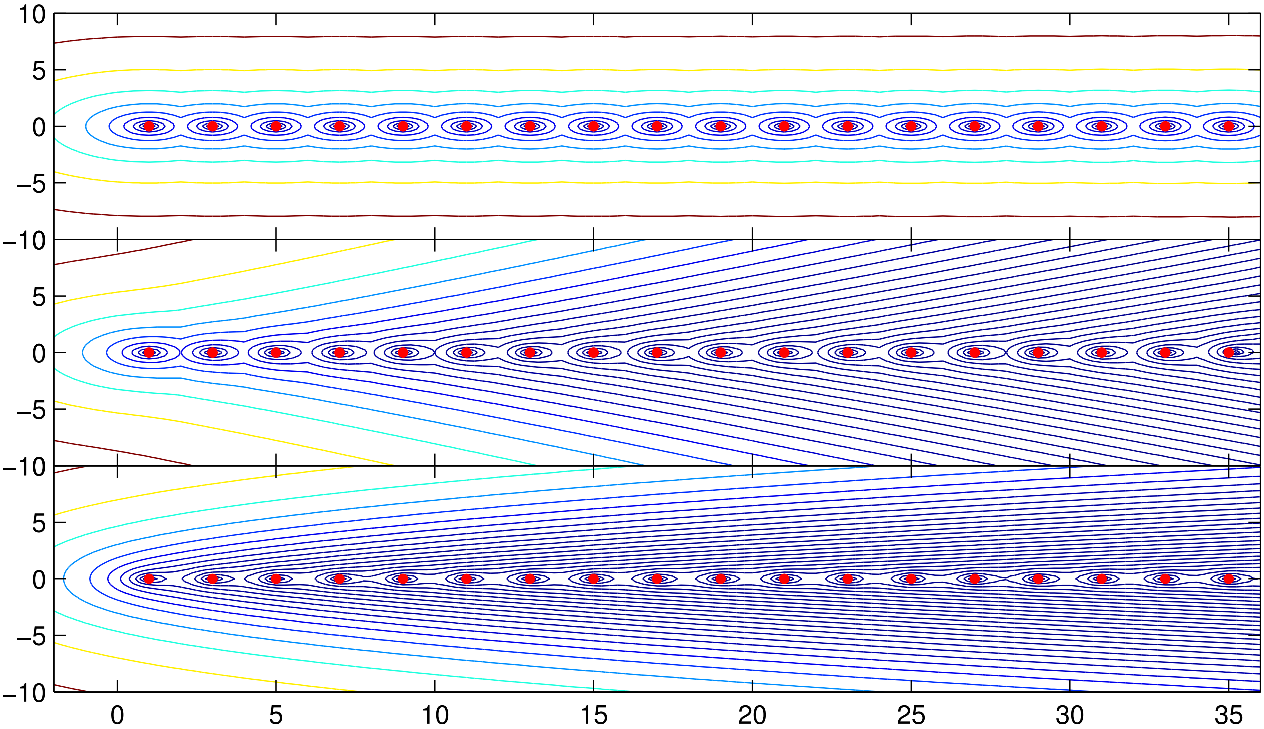

Figure 20.4: From top to bottom: Pseudospectra of the self-adjoint (20.32), rotated (20.35) with $\theta = \pi/4$ and shifted (20.38) harmonic oscillators which are formally conjugate to each other. Although the spectra (red dots) coincide in all these examples, the pseudospectra exhibit striking differences.

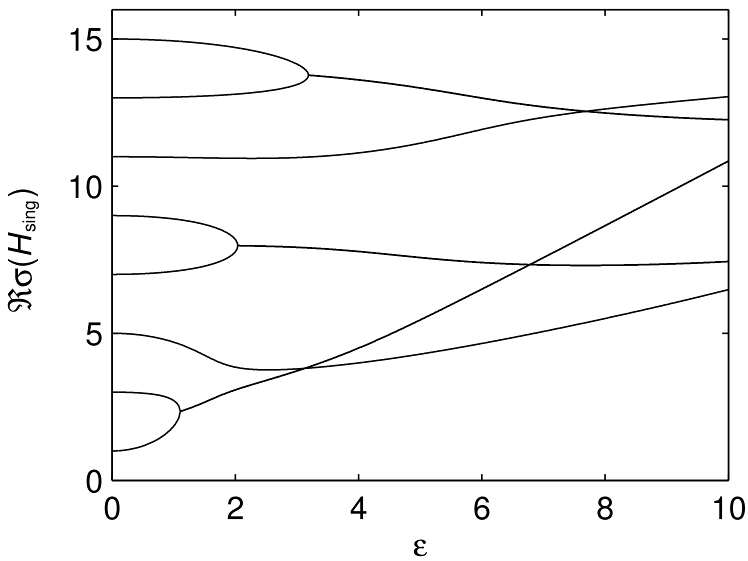

Figure 20.5: Real parts of eigenvalues of H with (20.40) as a function of ε.

• **Pseudospectrum.** Let us recall that the facts that the eigensystem contains a Riesz basis and the spectral properties described above imply that H is similar to a diagonal operator up to a possible finite number of finite dimensional Jordan blocks corresponding to the low lying eigenvalues. This in turn means that the pseudospectrum of H is trivial if there are no Jordan blocks. If λ_0 is a degenerate eigenvalue for which the algebraic multiplicity is strictly larger than the geometric one, the Jordan block result in a more singular behaviour of the resolvent, *i.e.*

$$\|(H-z)^{-1}\| \sim |\lambda_0 - z|^{-n}, \qquad n > 1,$$

around λ_0. This is visible in the plot of the pseudospectrum, since the peak around the degenerate eigenvalue λ_0 is wider, *i.e.* the level lines are further from λ_0, and we can call the pseudospectrum "almost trivial". We illustrate such a behaviour with the example

$$V(x) := i\varepsilon \left(\frac{1}{\sqrt{|x+1|}} - \frac{1}{\sqrt{|x-1|}} \right), \tag{20.40}$$

see Figure 20.6.

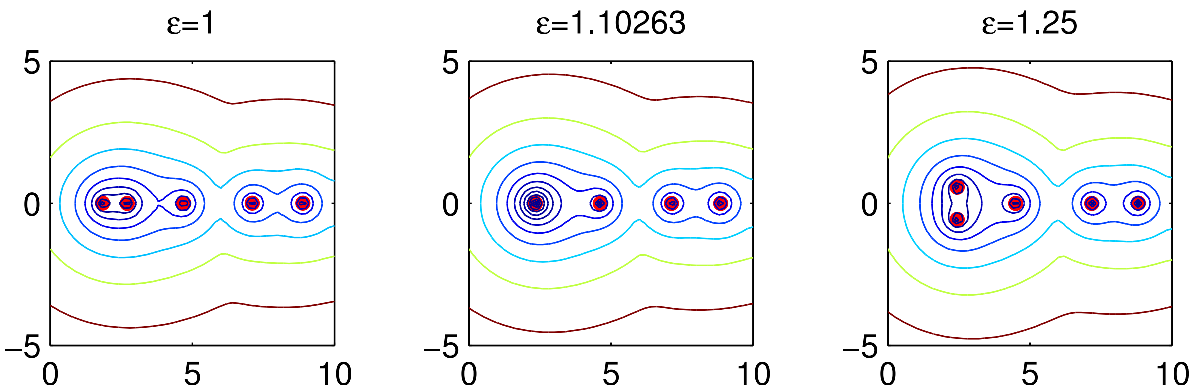

Figure 20.6: Pseudospectra around low lying eigenvalues of (20.40) for three increasing values of ε. From left to right: The simple eigenvalues (red dots) collide and create a Jordan block, then become again simple, but complex. The Jordan block structure is indicated by the wider peak around the degenerate eigenvalue.

Similar features appear in for instance a model on a finite interval with $\mathcal{PT}$-symmetric Robin boundary conditions, *cf* [47, 46, 48, 45], or for a $\mathcal{PT}$-symmetric square-well, *cf* [80, 70].

20.7.7 The gauged oscillator (Swanson's model)

We also study the operator

$$H := \omega\, a^* a + \alpha\, a^2 + \beta\, (a^*)^2 + \omega \quad \text{in} \quad L^2(\mathbb{R})\,, \tag{20.41}$$

introduced by Ahmed in [6] and later studied by Swanson in [75]. Here the creation and annihilation operators are defined in (20.34) (the reader is warned that a different convention is used in [75]) and ω, α, β are real parameters. It is assumed in [75] only that

$$\omega^2 - 4\alpha\beta \geq 0\,, \tag{20.42}$$

but we shall see that this condition is by far insufficient to make the results rigorous.

• **Rigorous definition of the operator.** First of all, we always assume $\omega \neq 0$ in order to define H as a perturbation of the harmonic oscillator H_{sa} defined in (20.32); without loss of generality, let us take $\omega > 0$. Second, we need to impose a condition on the smallness of α and β in order to ensure that the extra unbounded terms $r := \alpha\, a^2 + \beta\, (a^*)^2$ added in (20.41) to $\omega\, a^* a = \omega H_{\mathrm{sa}} - \omega$ do not completely change the character of the operator H_{sa}; see Section 20.7.8 for a discussion of the relevant condition in a more general setting.

Expressing annihilation and creation operators in terms of x and $\mathrm{d}/\mathrm{d}x$, we obtain an equivalent form

$$H = -(\omega+\alpha+\beta)\frac{\mathrm{d}^2}{\mathrm{d}x^2} + (\omega-\alpha-\beta)x^2 + (\alpha-\beta)(\frac{\mathrm{d}}{\mathrm{d}x}x + x\frac{\mathrm{d}}{\mathrm{d}x}) \quad \text{on} \quad L^2(\mathbb{R}). \tag{20.43}$$

We introduce H as an m-sectorial operator with compact resolvent under the condition

$$\omega - |\alpha+\beta| > 0. \tag{20.44}$$

Notice that this condition is stronger than (20.42) and it ensures that the real part of H indeed resembles the usual harmonic oscillator, because the constants in front of $-\mathrm{d}^2/\mathrm{d}x^2$ and x^2 are both positive.

We define a form

$$\begin{aligned} t[\psi] &:= (\omega+\alpha+\beta)\|\psi'\|^2 + (\omega-\alpha-\beta)\|x\psi\|^2 \\ &\quad + (\alpha-\beta)(\langle\psi', x\psi\rangle + \langle x\psi, \psi'\rangle), \\ \mathsf{D}(t) &:= \mathsf{D}(a) = \{\psi \in W^{1,2}(\mathbb{R}) \,|\, x\psi \in L^2(\mathbb{R})\}. \end{aligned} \tag{20.45}$$

Since the imaginary part of t satisfies

$$\begin{aligned}|\Im t[\psi]| &= |(\alpha-\beta)(\langle\psi', x\psi\rangle + \langle x\psi, \psi'\rangle)| \\ &\leq |\alpha-\beta|(\|\psi'\|^2 + \|x\psi\|^2) \\ &\leq \frac{|\alpha-\beta|}{\omega-|\alpha+\beta|}((\omega+\alpha+\beta)\|\psi'\|^2 + (\omega-\alpha-\beta)\|x\psi\|^2) \\ &= \frac{|\alpha-\beta|}{\omega-|\alpha+\beta|}\Re t[\psi],\end{aligned} \tag{20.46}$$

the form t is sectorial. Moreover, it is closed, since $\Re t$ is closed on the given domain. The operator H is then defined via the first representation theorem, *cf* [44, Thm. VI.2.1], as the unique m-sectorial operator associated with t. The operator H has a compact resolvent, which follows from [44, Thm. VI.3.3] and the fact that $\Re H$ has a compact resolvent; notice that $\Re H$ is an operator associated with $\Re t$ and it can be verified that

$$\Re H = -(\omega+\alpha+\beta)\,\frac{\mathrm{d}^2}{\mathrm{d}x^2} + (\omega-\alpha-\beta)\,x^2,$$

as expected.

• **Spectrum and pseudospectrum.** Since the resolvent of H is compact, the spectrum of H is discrete. To find the eigenvalues of H, we observe that H is *formally* similar to a self-adjoint harmonic oscillator. Indeed, substituting (20.34) to (20.41) and completing the square, we find

$$H = -(\omega-\alpha-\beta)\left(\frac{\mathrm{d}}{\mathrm{d}x} + \frac{\beta-\alpha}{\omega-\alpha-\beta}\,x\right)^2 + \frac{\omega^2-4\alpha\beta}{\omega-\alpha-\beta}\,x^2\,. \tag{20.47}$$

From this formula it is clear that H is self-adjoint if, and only if, $\alpha=\beta$. For $\alpha\neq\beta$, H is neither self-adjoint nor $\mathcal{T}$-self-adjoint, but it is $\mathcal{PT}$-symmetric and in fact real. The difference $\alpha-\beta$ acts as a sort of imaginary magnetic field. The magnetic field can be gauged out in one dimension; employing the same gauge transform for our "imaginary magnetic field," we *formally* check that $\tilde{H}_{\mathrm{sa}} = \Omega H \Omega^{-1}$ with

$$\tilde{H}_{\mathrm{sa}} := -(\omega-\alpha-\beta)\,\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{\omega^2-4\alpha\beta}{\omega-\alpha-\beta}\,x^2\,, \qquad \Omega := \exp\left(\frac{\beta-\alpha}{\omega-\alpha-\beta}\,\frac{x^2}{2}\right)$$

The word "formal" refers again to the fact that Ω is unbounded. Nevertheless, the similarity relation $\tilde{H}_{\mathrm{sa}} = \Omega H \Omega^{-1}$ is well defined on eigenfunctions of $\tilde{H}_{\mathrm{sa}}$ and we can deduce that

$$\sigma(H) = \sigma(\tilde{H}_{\mathrm{sa}}) = \left\{ (2k+1)\sqrt{\omega^2-4\alpha\beta} \;\middle|\; k=0,1,\dots \right\},$$

since eigenfunctions of H are complete in $L^2(\mathbb{R})$. The latter can be verified by adapting the standard proof of completeness of Hermite functions; see *e.g.* [17, Ex. 2.2.3].

Large pseudoeigenvalues can be shown to exist by applying Theorem 20.1, as before. Employing the unitary transform (20.25), we introduce a semiclassical analogue of H via $\mathcal{U}H\mathcal{U}^{-1} = \sigma^2 H_h$, where H_h is (20.47) with the small number $h := \sigma^{-2}$ put in front of the derivative. For the symbol f associated with H_h we get

$$\{f,\bar{f}\} = 8i(\alpha-\beta)\left[(\omega+\alpha+\beta)\,\xi^2 - (\omega-\alpha-\beta)\,x^2\right].$$

Consequently, Λ has the same structure as that of the rotated harmonic oscillator: a cone in the right complex half-plane with two semiaxes removed. Applying Theorem 20.1, we see that there is exponentially rapid resolvent growth in the interior of the cone. Again, for any $\varepsilon > 0$ there are complex points with positive real part, non-zero imaginary part, and large magnitude that lie in the pseudospectrum $\sigma_\varepsilon(H)$.

Although the straightforward application of Theorem 20.1 already shows non-trivial character of the pseudospectrum, there is significantly more structure to be found. In fact, we show that H is unitarily equivalent to a certain rotated harmonic oscillator, discussed in Section 20.7.4, and therefore information on the pseudospectrum and basis properties of eigenfunctions can be transferred directly to Swanson's model. Such a unitary equivalence is not a special property of this particular model; see Section 20.7.8.

In our particular case, a suitable unitary transform for H reads

$$\begin{aligned}\mathcal{U} &:= \mathcal{U}_1\mathcal{U}_2\mathcal{U}_3, \\ (\mathcal{U}_1\psi)(x) &:= e^{-i\delta x^2/2}\psi(x), \\ (\mathcal{U}_2\psi)(x) &:= (\mathcal{F}^{-1}e^{-i\xi^2/(4\delta)}\mathcal{F}\psi)(x), \\ (\mathcal{U}_3\psi)(x) &:= (2\delta)^{1/4}\psi((2\delta)^{1/2}x),\end{aligned} \tag{20.48}$$

where $\delta := (\omega+\alpha+\beta)^{1/2}(\omega-\alpha-\beta)^{-1/2}$ and $\mathcal{F}$ is the unitary Fourier transform

$$\mathcal{F}u(\xi) = \frac{1}{\sqrt{2\pi}} \int_{\mathbb{R}} e^{-ix\xi}\, u(x)\,\mathrm{d}x, \quad u \in L^1(\mathbb{R}) \cap L^2(\mathbb{R}). \tag{20.49}$$

The key steps are the relations for $\mathcal{U}_2^*\mathcal{U}_1^* x \mathcal{U}_1\mathcal{U}_2$ and $\mathcal{U}_2^*\mathcal{U}_1^* p \mathcal{U}_1\mathcal{U}_2$. Several straightforward manipulations and properties of $\mathcal{F}$ yield that for any $\varphi \in \mathscr{S}(\mathbb{R})$

$$\mathcal{U}_2^*\mathcal{U}_1^* x \mathcal{U}_1\mathcal{U}_2\varphi = \left(x - \frac{i}{2\delta}\frac{\mathrm{d}}{\mathrm{d}x}\right)\varphi, \quad \mathcal{U}_2^*\mathcal{U}_1^* p \mathcal{U}_1\mathcal{U}_2\varphi = \left(-\frac{i}{2}\frac{\mathrm{d}}{\mathrm{d}x} - \delta x\right)\varphi. \tag{20.50}$$

The latter implies

$$\mathcal{U}_2^*\mathcal{U}_1^* H \mathcal{U}_1\mathcal{U}_2 = \zeta\left(-\frac{1}{2\delta}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + 2\delta\frac{\overline{\zeta}}{\zeta}x^2\right) \tag{20.51}$$

with $\zeta := \sqrt{\omega^2 - (\alpha+\beta)^2} + i(\alpha-\beta)$. The additional rescaling $\mathcal{U}_3$ finally gives a multiple of the rotated harmonic oscillator:

$$\mathcal{U}^* H \mathcal{U} = \zeta\left(-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \frac{\overline{\zeta}}{\zeta}x^2\right). \tag{20.52}$$

The unitary equivalence shows that the eigenvectors of H do not form a basis and the norms of the spectral projections grow as in (20.37) with an appropriately chosen θ. Moreover, the numerically computed pseudospectra for H correspond to those for the rotated oscillator in Figure 20.4 after the appropriate adjustment of parameters. As in previous examples, the existence of non-trivial pseudospectra makes H very different from any self-adjoint operator, despite the reality of its spectrum and a formal similarity to a self-adjoint operator. In particular, the spectrum is highly unstable under small perturbations.

20.7.8 Elliptic quadratic operators

To better understand and extend the reduction (20.52) applied to the gauged oscillator, we now discuss general operators which are quadratic in $(x, \mathrm{d}/\mathrm{d}x)$. We begin with a quadratic symbol $q : \mathbb{R}^2 \to \mathbb{C}$,

$$q(x,\xi) := \alpha x^2 + 2\beta x\xi + \gamma\xi^2,$$

where the x variable represents the multiplication operator and the ξ variable represents the self-adjoint momentum operator $-i\,\mathrm{d}/\mathrm{d}x$ defined on $W^{1,2}(\mathbb{R})$. Such a representation necessarily involves a choice for $x\xi$ between $x(\mathrm{d}/\mathrm{d}x)$ and $(\mathrm{d}/\mathrm{d}x)x$; in the quadratic case, the *Weyl quantization* makes the choice

$$x\xi \mapsto \frac{1}{2}\left(x\Big(-i\frac{\mathrm{d}}{\mathrm{d}x}\Big) + \Big(-i\frac{\mathrm{d}}{\mathrm{d}x}\Big)x\right).$$

This choice ensures that real-valued q lead to self-adjoint operators, in addition to other convenient properties. (See, for instance, [31, Chap. 7] or [43, Sec. 18.5] for a far more general setting.)

We therefore arrive at the operator

$$\begin{aligned} Q &:= q^w(x,\xi) = \alpha x^2 - i\beta\left(x\frac{\mathrm{d}}{\mathrm{d}x} + \frac{\mathrm{d}}{\mathrm{d}x}x\right) - \gamma\frac{\mathrm{d}^2}{\mathrm{d}x^2}, \\ \mathsf{D}Q &:= \{u \in L^2(\mathbb{R}) \mid Qu \in L^2(\mathbb{R})\}. \end{aligned} \tag{20.53}$$

The characterization of the domain as the graph closure of the restriction to $\mathscr{S}(\mathbb{R})$ or $C_0^\infty(\mathbb{R})$ may be found in [42, pp. 425–426].

• **Ellipticity** It is natural to assume that $q(x,\xi)$ only vanishes at the origin:

$$q(x,\xi) = 0 \implies (x,\xi) = (0,0). \tag{20.54}$$

However, this is not sufficient to rule out degenerate behaviour of Q, and so one adds the assumption that

$$q(\mathbb{R}^2) \neq \mathbb{C}. \tag{20.55}$$

These conditions together assure us that there exists some nonzero complex number $\mu \in \mathbb{C}$ for which

$$\Re(\mu q(x,\xi)) \geq |(x,\xi)|^2 \tag{20.56}$$

and thus $\Re(\mu Q) = \frac{1}{2}(\mu Q + \overline{\mu} Q^*)$ acts like a harmonic oscillator.

If (20.54) holds but (20.55) fails, we find ourselves in a situation resembling that of a creation or annihilation operator (20.34) squared: either $\dim \mathsf{N}(Q - z) = 2$ for all $z \in \mathbb{C}$ or $\dim \mathsf{R}(Q - z)^\perp = 2$ for all $z \in \mathbb{C}$; see [58, Sec. 3.1]. This is precisely the situation which arises for the gauged oscillator, Section 20.7.7, when (20.42) holds but (20.44) fails.

Under (20.54) and (20.55), the spectral theory of the operator Q can be deduced from the spectral theory of the matrix sometimes called the *fundamental matrix*:

$$F := \begin{pmatrix} \beta & \gamma \\ -\alpha & -\beta \end{pmatrix}. \tag{20.57}$$

It is shown in [73, Prop. 3.3] that

$$\begin{aligned} \sigma(F) &= \pm\lambda, \\ \mathsf{N}(F \mp \lambda) &= \operatorname{span}\{(1, a_\pm)\}, \qquad \pm\Im a_\pm > 0. \end{aligned} \tag{20.58}$$

We note that, in dimension 1, we can identify $\mu = i/\lambda$ in (20.56) through choosing λ according to the signs of $\Im a_\pm$. Taking this notation into account, we then have from [73, Thm. 3.5] that

$$\sigma(Q) = \big\{ -i\lambda(2k+1) \bigm| k = 0, 1, 2, \ldots \big\}.$$

• **Linear symplectic transformations** One advantage of the Weyl quantization is that we may transform our symbols by composition with symplectic transformations; see *e.g.* [43, Sec. 18.5] for a detailed accounting of the theory. In our simplified (linear, dimension one) setting, the set of real linear symplectic transformations is simply the set of a 2-by-2 matrices with real entries and determinant equal to one. Any such matrix may be written [43, Lem. 18.5.8] as a composition of matrices of the form

$$G_b := \begin{pmatrix} 1 & 0 \\ b & 1 \end{pmatrix}, \quad V_c := \begin{pmatrix} c & 0 \\ 0 & 1/c \end{pmatrix}, \quad J := \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \tag{20.59}$$

with $b, c \in \mathbb{R}$ and $c \neq 0$.

What is more, one may transform a quadratic symbol by composing with such a matrix by conjugating with an easily-understood unitary transformation on $L^2(\mathbb{R})$. Specifically, we use multiplication by a complex Gaussian

$$\mathcal{G}_b u(x) := e^{ibx^2/2} u(x), \tag{20.60}$$

a scaling change of variables,

$$\mathcal{V}_c u(x) := c^{-1/2} u(x/c), \tag{20.61}$$

and the unitary Fourier transform (20.49). Using definition (20.53), it is then straightforward to check that

$$\begin{aligned} \mathcal{G}_b^* q^w(x,\xi) \mathcal{G}_b &= (q \circ G_b)^w(x,\xi), \\ \mathcal{V}_c^* q^w(x,\xi) \mathcal{V}_c &= (q \circ V_c)^w(x,\xi), \\ \mathcal{F}^* q^w(x,\xi) \mathcal{F} &= (q \circ J)^w(x,\xi). \end{aligned}$$

One important example is the change of variables which gives us the correspondence between high-energy and semiclassical limits: for any $z \in \mathbb{C}$,

$$q^w(x,\xi) - z = \mathcal{V}_{\sqrt{h}}^* \left(\frac{1}{h} (q^w(x, h\xi) - hz) \right) \mathcal{V}_{\sqrt{h}}. \tag{20.62}$$

Therefore the regime with spectral parameter rz as $r \to \infty$ for the operator $q^w(x,\xi)$ is unitarily equivalent to the regime with spectral parameter z fixed for the operator $\frac{1}{h} q^w(x, h\xi)$ as $h = 1/r \to 0^+$.

• **Reduction to rotated harmonic oscillator** In [57, Lem. 2.1], Pravda-Starov identifies a procedure for taking an elliptic quadratic form q and finding $\mu \in \mathbb{C}\backslash\{0\}$ and a real matrix T with $\det T = 1$ for which

$$(q \circ T)(x,\xi) = \mu \left((1 + i\lambda_1) x^2 + (1 + i\lambda_2) \xi^2 \right) \tag{20.63}$$

for $\lambda_1, \lambda_2 \in \mathbb{R}$. Applying a scaling like (20.62) and scaling μ allows us to assume that the coefficients of x^2 and ξ^2 have the same modulus. It is then evident that the resulting symbol is a multiple of that of a rotated harmonic oscillator (20.35).

If one wishes only to identify the parameters of the rotated harmonic oscillator involved, one may appeal to the spectral decomposition of the fundamental matrix and the growth of the spectral projections. An application of Corollary 1.7 in [79] in terms of the eigensystem (20.58) shows that the norm of the spectral projections P_k for the eigenvalues $(2k+1)\lambda/i$ obey the asymptotics

$$\lim_{k\to\infty} \frac{\log \|P_k\|}{k} = \frac{1}{2}\log\frac{1+|c_+|}{1-|c_+|}, \quad c_+ = -\frac{a_+ - \overline{a_-}}{a_+ - a_-}.$$

From (20.37), we see that this uniquely identifies a rotated harmonic oscillator with $\theta \geq 0$. The multiplicative factor, in turn, is determined by the ground state energy, that is, the eigenvalue corresponding to $k = 0$. We arrive at the following proposition.

Proposition 20.6. *Let Q be any quadratic operator as in* (20.53) *with symbol q. Assume that q is elliptic as in* (20.54) *and* (20.55)*, and therefore let the eigensystem of the fundamental matrix of q be as in* (20.58)*. Let $\theta \in [0, \pi/2)$ be determined by*

$$\sin\theta = \left|\frac{a_+ - \overline{a_-}}{a_+ - a_-}\right|.$$

Then Q, as an unbounded operator on $L^2(\mathbb{R})$, is unitarily equivalent to

$$\lambda\left(-e^{-i\theta}\frac{\mathrm{d}^2}{\mathrm{d}x^2} + e^{i\theta}x^2\right).$$

• **Higher dimension** The extension of the spectral and pseudospectral theory to elliptic quadratic operators in higher dimension is well-developed but not complete. We content ourselves with a brief description and references.

The Weyl quantization of a quadratic form

$$q(x,\xi) : \mathbb{R}^{2d} \to \mathbb{C}$$

in dimension $d \geq 2$ also associates the variable x_j with multiplication by x_j, associates the variable ξ_j with $-i\partial/\partial x_j$, and resolves the problem of commutativity (in the quadratic case) by taking an average:

$$(x_j\xi_j)^w u(x) = \frac{1}{2i}\left(x_j\frac{\partial}{\partial x_j}u(x) + \frac{\partial}{\partial x_j}(x_j u(x))\right).$$

The ellipticity hypothesis is simpler, since in dimension 2 or greater, (20.54) implies (20.55), shown in [73, Lem. 3.1].

Under the assumption (20.54), the spectrum of $Q = q^w(x,\xi)$ is a lattice determined by eigenvalues of the matrix corresponding to the fundamental matrix (20.57); the formula is given in [73, Thm. 3.5].

It was recently shown in [21] that, regardless of dimension, an elliptic quadratic form obeying a $\mathcal{PT}$-symmetry condition is *formally* similiar to a self-adjoint operator if and only if the spectrum is real and the fundamental matrix is diagonalizable. This similarity is only enacted eigenspace by eigenspace, and the authors observe that the pseudospectral considerations prevent the similarity transformations from being bounded with bounded inverse on $L^2(\mathbb{R}^d)$.

In [58], Pravda-Starov conducts a complete study of the semiclassical pseudospectrum for non-normal elliptic quadratic operators. It is shown in [58, Sec. 3.2] that, for a non-normal operator, the bracket condition is violated everywhere in the interior of the range of the symbol and therefore exponentially accurate pseudomodes exist.

Conversely, exponential upper bounds for the resolvent are proven in [41], except that exponential growth $C^{1/h}$ may need to be replaced by the more rapid growth $(C/h)^{C/h}$ when the fundamental matrix contains Jordan blocks.

Finally, the associated spectral projections for a non-normal quadratic operator were shown in [79] to usually increase at an exponential rate, though there are degenerate situations such as when Jordan blocks are present in the fundamental matrix.

20.7.9 Numerical computation of JWKB solutions

The proof of Theorem 20.1 proceeds by creating pseudomodes as JWKB (Jeffreys-Wentzel-Kramers-Brillouin) approximations for which $(H - z)u \approx 0$. Focusing on the one-dimensional Schrödinger case, these functions can be expressed using a few elementary operations, including differentiation and integration; see (20.67), (20.70),

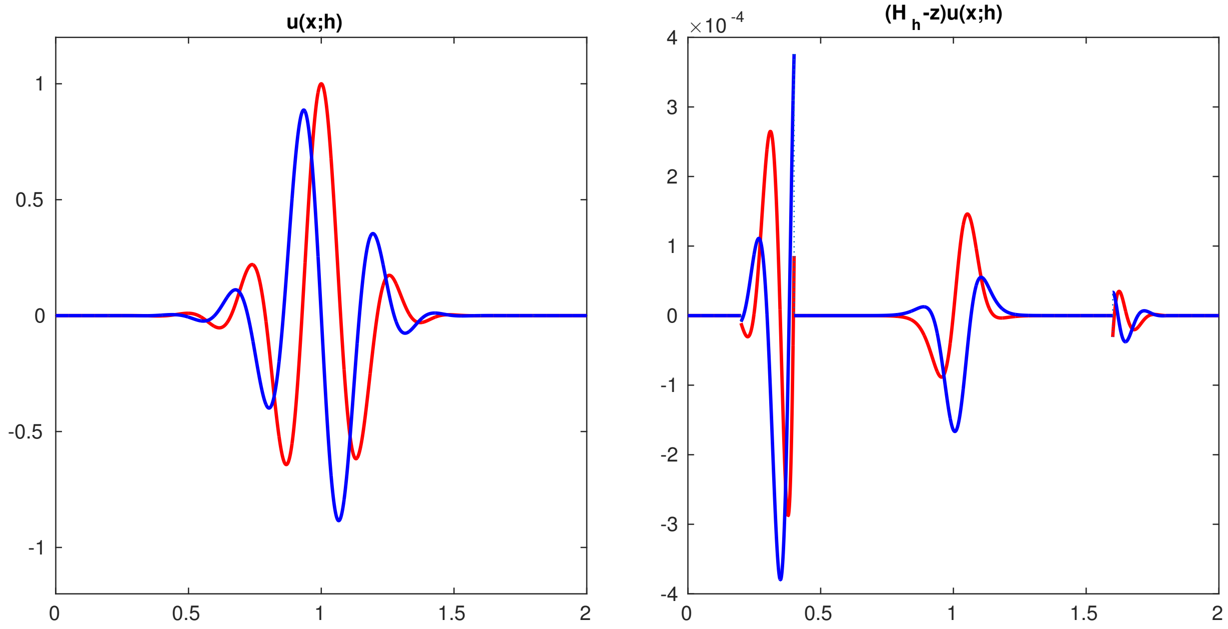

Figure 20.7: Pseudomode (left) and image (right) for semiclassical rotated harmonic oscillator. The red curve is the real part, and the blue the imaginary.

(20.72), and (20.73). The software package Chebfun [78] allows us to easily compute these pseudomodes with high accuracy.

In Figure 20.7 we compare a JWKB pseudomode for the semiclassical rotated harmonic oscillator

$$H_h = -h^2 e^{-i\pi/4} \frac{\mathrm{d}^2}{\mathrm{d}x^2} + e^{i\pi/4} x^2 \tag{20.64}$$

discussed in Section 20.7.4 with $z = e^{-i\pi/4}(1/2 + i)$, $h = 2^{-5}$, and

$$u(x;h) = \chi(x) e^{i\varphi(x)/h} \sum_{j=0}^{6} h^j a_j(x).$$

The plot on the left is of the real part (red) and the imaginary part (blue) of the pseudomode, and the plot on the right is of the image, $(H_h - z)u$. One may compute that

$$\frac{\|(H_h - z)u\|}{\|u\|} \approx 2.5041 \times 10^{-4}.$$

One can clearly see the contributions from the gradient of the support of the cutoff function, which is $[0.2, 0.4] \cup [1.6, 1.8]$.

If one studies instead the semiclassical rescaling of the shifted harmonic oscillator

$$H_h = -h^2 \frac{\mathrm{d}^2}{\mathrm{d}x^2} + x^2 + 2ih^{1/2}x - h \tag{20.65}$$

discussed in Section 20.7.5 we have noticeable but less accurate pseudomodes, with the principal error given on the support of the cutoff function. In Figure 20.8, one has a similar JWKB solution and its image with $h = 2^{-8}$, $z = 2 - h + 2ih^{1/2}$, and

$$u(x;h) = \chi(x) e^{i\varphi(x)/h} \sum_{j=0}^{2} h^j a_j(x).$$

(We may see numerically that there is practically no difference in norms when taking one, two, or ten terms in the expansion.) Since h is very small, the JWKB function oscillates quite rapidly, and since the decay of $e^{i\varphi/h}$ is comparatively weak, the principal error comes from the cutoff function, whose gradient is again supported on $[0.2, 0.4] \cup [1.6, 1.8]$. We have here

$$\frac{\|(H_h - z)u\|}{\|u\|} \approx 2.0290 \times 10^{-3}.$$

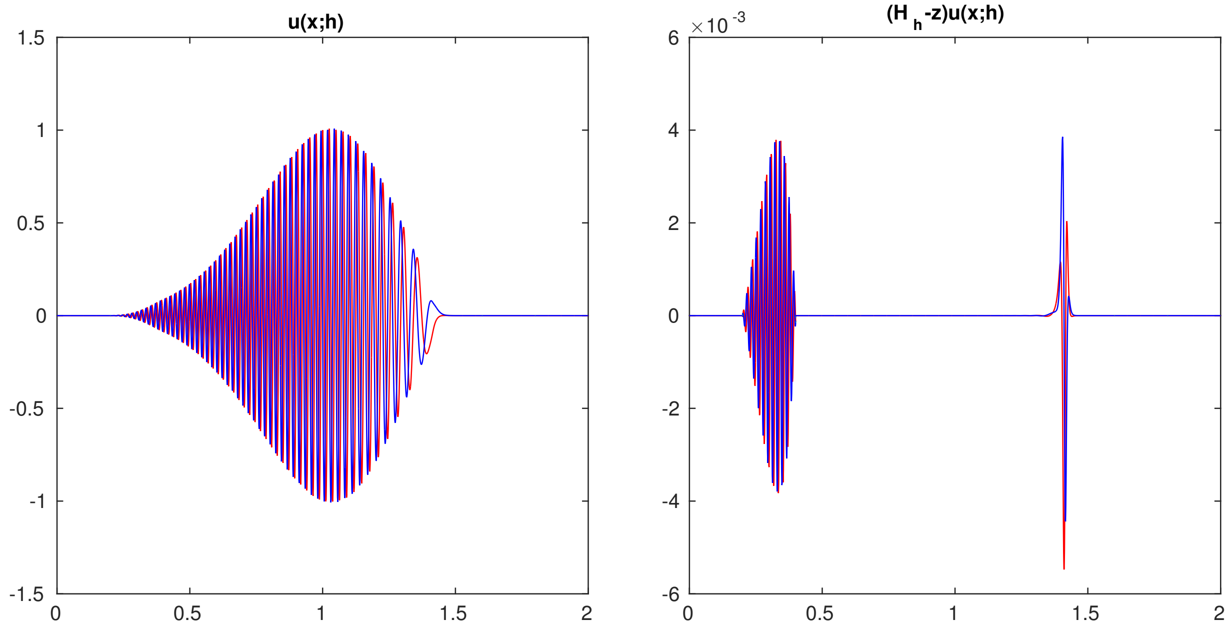

Figure 20.8: Pseudomode (left) and image (right) for semiclassical rescaling of shifted harmonic oscillator. The red curve is the real part, and the blue the imaginary.

We can then compare the accuracy of the $L^2(\mathbb{R})$-normalized pseudomodes by plotting $\|(H_h - z)u\|$ versus $1/h$ for a variety of h, presented in Figure 20.9. On the left, we have the norms for the semiclassical rotated harmonic oscillator (20.64) at $z = 1 + 4i$, and on the right, we have those for the rescaled shifted harmonic oscillator (20.65) at $z = 2 - h + 2ih^{1/2}$. We can observe that the norm ratios for the pseudomodes for the rotated harmonic oscillator decrease like $\exp(-c/h)$ while those for the shifted harmonic oscillator decrease more slowly.

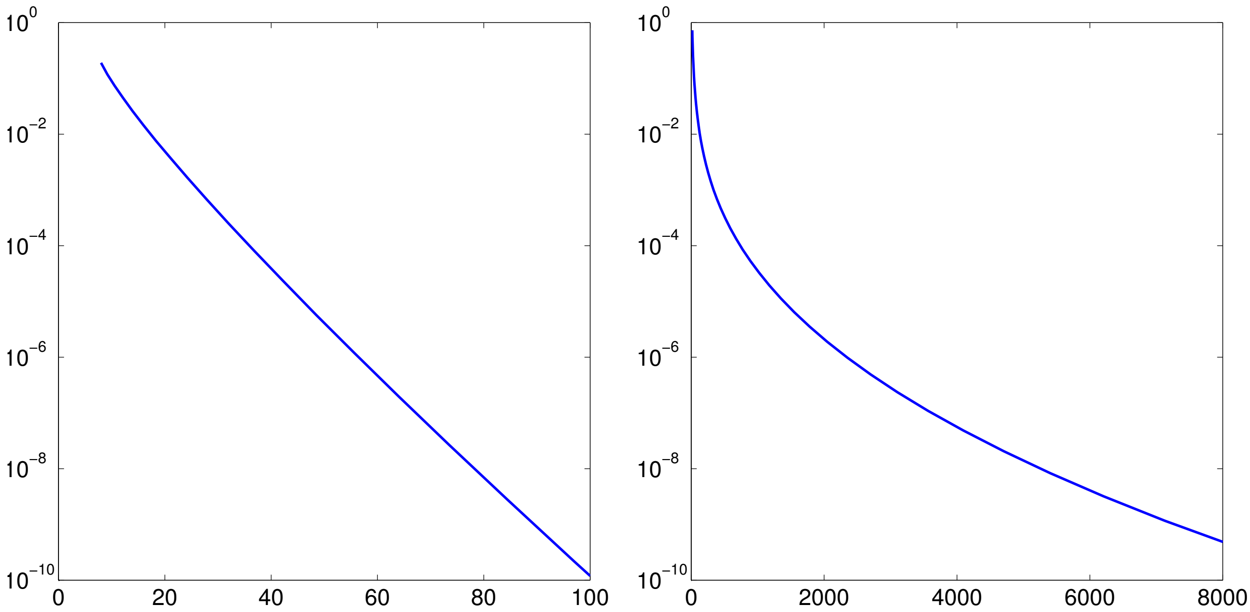

Figure 20.9: $\|(H_h - z)u\|$ as a function of $1/h$ for normalized pseudomodes for rotated harmonic oscillator (left) and shifted harmonic oscillator (right).

20.8 Appendix: Existence proofs for pseudomodes

For the interested reader, we include detailed proofs of Theorem 20.1 in the case of a Schrödinger operator and of Theorem 20.2. In these proofs, the constant $C > 0$ may change from line to line. Furthermore, we understand semiclassical statements involving h to only hold for $h \in (0, h_0]$ for some $h_0 > 0$; so long as h_0 changes only finitely many times in the proof, we are allowed to make conclusions "for h sufficiently small" in our theorems.

20.8.1 Proof of special case of Theorem 20.1

We restrict our attention to the case

$$H_h = -h^2 \frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x).$$

The symbol of H_h is

$$f(x, \xi) = \xi^2 + V(x), \tag{20.66}$$

and

$$\frac{1}{2i} \{f, \bar{f}\} = -2\xi \Im V'(x).$$

Therefore $z \in \Lambda$, defined in (20.15), if and only if there exists $(x_0, \xi_0) \in \mathbb{R}^2$ with $z = \xi_0^2 + V(x_0)$, $\Im V'(x_0) \neq 0$, and $-\xi_0 \Im V'(x_0) > 0$. Equivalently, since we may choose the sign of ξ_0, there exists some $x_0 \in \mathbb{R}$ where $\Im V'(x_0) \neq 0$ and $z - V(x_0)$ is a positive real number. We only need to assume that $V(x)$ is analytic in a neighborhood of x_0.

After a translation, we may assume that $x_0 = 0$. We seek a JWKB approximation (see for instance [31, Chap. 2]) to a solution of $(H_h - z)u = 0$ of the form

$$u(x; h) = e^{i\varphi(x)/h} \sum_{j=0}^{N(h)} h^j a_j(x) \tag{20.67}$$

for $a_j(x)$ analytic near $x_0 = 0$. The strategy is to choose the phase function such that conjugation by the multiplication operator $e^{-i\varphi(x)/h}$ reduces H_h to a transport equation plus an error in h. The functions a_j may be found iteratively and then $N(h)$ may be chosen to give an accurate local solution. The quasimode will then be obtained by multiplying $u(x; h)$ by a fixed cutoff function χ localizing to a neighborhood of $x_0 = 0$. An important difference making the JWKB theory for non-self-adjoint operators somewhat simpler is that the phase function $\varphi(x)$ has a significant imaginary part. This allows for multiplication by cutoff functions with small errors, a technique which is generally not available for self-adjoint operators where φ is real-valued.

We require that the phase function $\varphi(x)$ satisfies the eikonal equation

$$f(x, \varphi'(x)) - z = 0$$

for f from (20.66). Clearly this implies that $\varphi'(x) = \pm\sqrt{z - V(x)}$. Since $z - V(0) > 0$, this function is analytic in a neighborhood of $0 \in \mathbb{C}$.

We allow the sign to be determined by the bracket condition

$$\frac{1}{2i}\{f, \bar{f}\}(x, \xi) = -2\Im V'(x)\xi > 0. \tag{20.68}$$

Applying this to $(x, \xi) = (0, \varphi'(0))$ indicates that the sign of $\varphi'(0)$ should be taken to be the opposite of the sign of $\Im V'(0)$. Alternately, the importance of this choice of sign may be seen by observing that

$$\varphi''(x) = -\frac{V'(x)}{2\varphi'(x)} \tag{20.69}$$

and thus our choice is made so that $\Im \varphi''(0) > 0$, which means that $e^{i\varphi(x)/h}$ has rapid decay away from $x = 0$. We arrive at the formula

$$\varphi(x) = -\operatorname{sgn}(\Im V'(x_0)) \int_0^x \sqrt{z - V(y)}\, \mathrm{d}y. \tag{20.70}$$

We may then check that

$$e^{-i\varphi/h}(H_h - z)e^{i\varphi/h} = \frac{2h}{i}(\varphi' \frac{\mathrm{d}}{\mathrm{d}x} + \frac{1}{2}\varphi'') - h^2 \frac{\mathrm{d}^2}{\mathrm{d}x^2}.$$

So long as $\{a_j\}_{j=0}^{\infty}$ satisfy the transport equations

$$\varphi'(x)a_0'(x) + \frac{1}{2}\varphi''(x)a_0(x) = 0$$

and

$$\varphi'(x)a_j'(x) + \frac{1}{2}\varphi''(x)a_j(x) = \frac{i}{2}a_{j-1}''(x), \quad j = 1, 2, \dots,$$

we have

$$e^{-i\varphi/h}(H_h - z)e^{i\varphi/h}\left(\sum_{j=0}^{N} h^j a_j\right) = -h^{N+2}a_N''. \tag{20.71}$$

We are free to choose $a_0(0) = 1$ and $a_j(0) = 0$ for all $j > 0$. Using the integrating factor $\exp(\int_0^x \varphi''(y)/(2\varphi'(y))\,\mathrm{d}y) = C\sqrt{\varphi'(x)}$ immediately gives that

$$a_0(x) = \frac{\sqrt{\varphi'(0)}}{\sqrt{\varphi'(x)}} \tag{20.72}$$

and that, for $j > 0$,

$$a_{j+1}(x) = \frac{1}{\sqrt{\varphi'(x)}} \int_0^x \frac{ia_j''(y)}{2\sqrt{\varphi'(y)}}\,dy. \tag{20.73}$$

We note that, in a sufficiently small neighborhood of zero in the complex plane, φ' may be extended to an analytic function which is bounded away from zero, and therefore each a_j is certainly analytic on that neighborhood of zero.

We now consider bounds on the functions a_j. As in Example 1.1 of [74], we will show that the a_j obey the estimates

$$|a_j(z)| \leq C_1^{j+1} j^j \tag{20.74}$$

for some $C_1 > 0$ and all z in a neighborhood of the origin. A sequence of functions satisfying these estimates is said to be a *formal analytic symbol*. Once these bounds are established, we may define the h-dependent function

$$a(z; h) = \sum_{0 \leq j \leq (eC_1 h)^{-1}} h^j a_j(z), \tag{20.75}$$

summing over a collection of j chosen such that

$$|h^j a_j(z)| \leq C_1(C_1 h j)^j \leq C_1 e^{-j}. \tag{20.76}$$

Since $\{e^{-j}\}_{j \geq 0}$ is summable, we will therefore have that $\{a(z; h)\}_{0 < h \leq h_0}$ is a uniformly bounded collection of analytic functions on the set where (20.74) holds.

The natural norm to use here for analytic functions is the supremum norm, so for $K \subseteq \mathbb{C}$ we write

$$\|g\|_K = \sup_{z \in K} |g(z)|.$$

For balls in the complex plane centered at zero, we use the notation

$$B(R) = \left\{ z \in \mathbb{C} \;\middle|\; |z| < R \right\}.$$

Fix $R_0 > 0$ such that, on $B(R_0)$, the phase function φ is analytic, the modulus of the derivative $|\varphi'|$ is bounded from above and below, and $\Im\varphi''(x) > 1/C$ for some $C > 0$.

Cauchy's estimates for the second derivative of a analytic bounded function g defined on $B(R)$ read

$$|g''(z)| \leq \frac{2\|g\|_{B(R)}}{(R - |z|)^2}. \tag{20.77}$$

We integrate the estimates applied to a_j'' to obtain bounds for a_{j+1}:

$$\begin{aligned}
|a_{j+1}(z)| &= \left| \frac{1}{\sqrt{\varphi'(z)}} \int_0^z \frac{ia_j''(\zeta)}{2\sqrt{\varphi'(\zeta)}}\,d\zeta \right| \\
&\leq \|(\varphi')^{-1}\|_{B(R)} \int_0^{|z|} \frac{\|a_j\|_{B(R)}}{(R - t)^2}\,\mathrm{d}t \\
&\leq \|(\varphi')^{-1}\|_{B(R)} \|a_j\|_{B(R)} \left(\frac{1}{R - |z|} - \frac{1}{R} \right) \\
&= \frac{|z|}{R(R - |z|)} \|(\varphi')^{-1}\|_{B(R)} \|a_j\|_{B(R)}.
\end{aligned} \tag{20.78}$$

The estimate for $|a_{j+1}(z)|$ is stronger than the usual Cauchy's estimate for the first derivative when z is near zero, which corresponds to having set $a_{j+1}(0) = 0$.

To obtain the estimates (20.74) on $B(R_0/2)$, we fix $j > 0$ and iterate (20.78) on balls of radius

$$R_k = \left(1 - \frac{k}{2j}\right) R_0, \quad k = 0, \ldots, j-1.$$

When $|z| \le R_{k+1}$, we have

$$\frac{|z|}{R_k(R_k - |z|)} \le \frac{|z|}{R_k(R_k - R_{k+1})} = \frac{|z|}{(R_0/2)(R_0/2j)} \le \frac{4j|z|}{R_0^2},$$

since $R_k > R_0/2$ when $k < j$. Therefore we may bound a_{k+1} on the disc of radius R_{k+1} using a bound for a_k on the disc of radius R_k and (20.78):

$$\begin{aligned} \|a_{k+1}\|_{B(R_{k+1})} &\le \frac{|z|}{R_k(R_k - |z|)} \|(\varphi')^{-1}\|_{B(R_k)} \|a_k\|_{B(R_k)} \\ &\le \frac{4j|z|}{R_0^2} \|(\varphi')^{-1}\|_{B(R_0)} \|a_k\|_{B(R_k)}. \end{aligned} \tag{20.79}$$

Therefore, when $j > 0$, we take the product of the estimates (20.79) for $k = 0, \ldots, j-1$ to obtain

$$\|a_j\|_{B(R_0/2)} \le \|a_0\|_{B(R_0)} \left(C_2|z|j\right)^j, \quad C_2 = \frac{4}{R_0^2} \|(\varphi')^{-1}\|_{B(R_0)}. \tag{20.80}$$

The estimate (20.74) on $B(R_0/2)$ immediately follows, with

$$C_1 = \max\left(\|a_0\|_{B(R_0)}, \frac{2}{R_0} \|(\varphi')^{-1}\|_{B(R_0)}\right). \tag{20.81}$$

Having established estimates for $a(z; h)$ when $z \in B(R_0/2)$, let $\chi \in C_0^\infty(\mathbb{R})$ be equal to one in a neighborhood of $0 \in \mathbb{R}$ and have support in a compact subset of the interval $(-R_0/2, R_0/2)$. We then define our pseudomode as

$$u(x; h) = e^{i\varphi(x)/h} \chi(x) a(x; h),$$

with $a(x; h)$ defined in (20.75).

We then estimate the $L^2(\mathbb{R})$ norm

$$\|H_h - z)u(x; h)\| \le \|\chi(H_h - z)e^{i\varphi/h} a\| + \|[(H_h - z), \chi]e^{i\varphi/h} a\| \tag{20.82}$$

as follows. First, we recall that we have chosen R_0 such that $\Im\varphi''(x) > 1/C_3$ for some $C_3 > 0$. Since $\varphi(0) = 0$ and $\varphi'(0)$ is real, we therefore have that

$$|e^{i\varphi(x)/h}| \le \exp\left(-\frac{1}{2C_3 h} x^2\right), \quad \forall x \in \operatorname{supp}\chi. \tag{20.83}$$

Since $|e^{-i\varphi/h}| \ge 1$ on $\operatorname{supp}\chi$, we may multiply by $e^{-i\varphi/h}$ and use (20.71) to obtain

$$\|\chi H_h e^{i\varphi/h} a\| \le \|\chi e^{-i\varphi/h} H_h e^{i\varphi/h} a\| = \|h^{N+2} a_N''(x)\chi(x)\|,$$

with $N = N(h) = \lfloor (eCh)^{-1} \rfloor$. Cauchy's estimates (20.77) along with (20.76) show that $h^{N+2} a_N''(x) \le Ce^{-1/(Ch)}$ for $C > 0$ independent of h and all $x \in \operatorname{supp}\chi$. We therefore have, for some $C > 0$, the estimate

$$\|\chi H_h e^{i\varphi/h} a\| \le Ce^{-1/(Ch)}.$$

In the commutator of $(H_h - z)$ and χ, only the derivatives in H_h play a role. We compute

$$\begin{aligned} [(H_h - z), \chi]\, e^{i\varphi/h} a &= \left[-h^2 \frac{\mathrm{d}^2}{\mathrm{d}x^2}, \chi\right] e^{i\varphi/h} a \\ &= -h^2 e^{i\varphi/h} \left(\chi'' a + 2\chi' \left(a' + \frac{i\varphi'}{h} a\right)\right). \end{aligned} \tag{20.84}$$

On $\operatorname{supp}(\chi)$, we have uniform bounds on a by (20.76) and therefore on a' by Cauchy's estimates. As before, φ' is controlled by the choice of R_0. Exponential decay comes from the fact that $\operatorname{supp}(\chi')$ avoids a neighborhood of 0: by (20.83), we have that

$$|e^{i\varphi(x)/h}| \le e^{-1/(Ch)}, \quad \forall x \in \operatorname{supp}(\chi'). \tag{20.85}$$

Therefore the second term in (20.82) is also exponentially small in $1/h$.

Having proven that both terms in (20.82) are exponentially small, the proof is complete upon showing that $u(x;h)$ is not exponentially small. Intuitively, this is clear from the choice of φ and that $a_0(0)=1$ and $a_j(0)=0$ for $j>0$, from which we know that $u(x;h)$ resembles $e^{-\varphi''(0)x^2/(2h)}$ in a small neighborhood of zero. Formally, since (20.80) gives $|h^j a_j(z)| \le C(C|z|)^j$ for $|z|<R_0/2$ and $0<j\le N(h)=(eC_1h)^{-1}$, we have for some $r_0>0$ sufficiently small the estimate

$$\left\| \sum_{j=1}^{N(h)} h^j a_j(z) \right\|_{B(r)} \le Cr, \quad 0<r\le r_0.$$

Since $a_0(z)$ is close to 1 and $\Im\varphi(z)$ is close to $\frac{1}{2}\Im\varphi''(0)z^2$ when z is close to 0, we can consider r sufficiently small and fixed to obtain

$$\|u(x;h)\| \ge \|u(x;h)\|_{L^2((-r,r))} \ge \frac{1}{C}\left(\int_{-r}^{r} \exp\left(\frac{1}{Ch}x^2\right)\,dx\right)^{1/2} \ge \frac{1}{C}h^{1/4}$$

when h is sufficiently small.

Since we have shown that $\|H_h u(x;h)\| \le Ce^{-1/(Ch)}$ and $\|u(x;h)\| \ge h^{1/4}/C$, this completes the proof of the theorem in this special case. ◻

• **Uniformity on compact sets.** We also remark that the exponential resolvent growth may generally be made uniform on compact subsets of Λ, the interior of the semiclassical pseudospectrum defined in (20.15). In the case of the Schrödinger operator, for any $z\in\Lambda$ we may take x_0 with $\Im V(x_0)=\Im z$ and define the phase function

$$\varphi(x) = \pm\int_{x_0}^{x} \sqrt{z-V(y)}\,\mathrm{d}y,$$

with the sign chosen so that $\Im\varphi''(x_0)>0$.

The exponentially rapid resolvent growth then follows from having $C>0$ and $R_1>R_0>0$ for which the estimates

$$|x-x_0|<R_1 \implies \frac{1}{C} \le |\varphi'(x)| \le C \tag{20.86}$$

and

$$R_0<|x-x_0|<R_1 \implies \Im\varphi(x) \ge \frac{1}{C} \tag{20.87}$$

hold: the former gives (20.74) by way of (20.81) and the latter gives (20.85), which are together sufficient to prove exponential growth of the resolvent.

The condition $\Im V'(x_0)\neq 0$ means that x_0 may be chosen locally as a continuous function of $\Im z$; it is then a simple matter to verify that (20.86) holds with uniform constants in a neighborhood of $z\in\Lambda$. Local uniformity of (20.87) then follows from $\Im\varphi''(x_0)>0$.

20.8.2 Proof of Theorem 20.2

As usual, we may make the change of variables $y=h^{-1/2}x$, arriving at an operator unitarily equivalent to hH_h:

$$\tilde{H}_h = -h^2\frac{\mathrm{d}^2}{\mathrm{d}y^2} + y^2 + 2ih^{1/2}y - h \simeq hH_h.$$

We will let $h^{-1}=\Re z$ so that

$$H_h - z \simeq h^{-1}(\tilde{H}_h-(1+it)), \quad t=\frac{\Im z}{\Re z}.$$

In this case, we have a symbol

$$\tilde{f}(y,\eta) = \eta^2+y^2+2ih^{1/2}y-h,$$

and so we cannot directly apply the results of [29]. We can, however, adapt the previous proof.

We can see that $1+it=\tilde{f}(y_0,\eta_0)$ for some $(y_0,\eta_0)\in\mathbb{R}^2$ if and only if

$$1+h=\eta_0^2+y_0^2, \quad t=2ih^{1/2}y_0,$$

implying that $|y_0|\le 1+h$ and

$$|t| \le 2h^{1/2}(1+h).$$

The eikonal equation $\tilde{f}(y, \varphi'(y)) = 0$ is then solved by integrating

$$\begin{aligned}\varphi'(y) &= -\sqrt{(1+h+it) - ih^{1/2}y - y^2} \\ &= -(1+h-y^2)\left(1 + \frac{i(t-2h^{1/2}y)}{1+h-y^2} + \mathcal{O}\left(\left(\frac{t-2h^{1/2}y}{1+h-y^2}\right)^2\right)\right).\end{aligned}$$

As usual, we choose the sign of the square root to satisfy a bracket condition like (20.68).

To ensure that, on a uniform neighborhood of y_0, the phase $\varphi'(y)$ is analytic and there exists $C > 0$ for which $1/C \leq |\varphi'(y)| \leq C$, we must assume that $1 + h - y^2$ is bounded away from zero by a constant. We therefore assume that $|y_0| < 1 - \varepsilon$ for some $\varepsilon > 0$. We remark that this is connected to assuming that $1 + it$ is in the interior of the range of the symbol. The scaling argument shows that this assumption is equivalent to the hypothesis that

$$\Im z \leq 2\left(1 - \varepsilon + (\Re z)^{-1}\right)\sqrt{\Re z}.$$

The term $(\Re z)^{-1}$ is negligible as $\Re z \to \infty$.

Note that

$$\varphi''(y) = \frac{-ih^{1/2} - y}{\varphi'(y)}$$

and so, since we chose the sign of the square root to have $\varphi'(y_0) < 0$, we have

$$\frac{1}{C}\sqrt{h} \leq \Im\varphi''(y) \leq C\sqrt{h}$$

on a sufficiently small but fixed neighborhood.

We may then construct exponentially accurate approximations to a solution of

$$e^{-i\varphi/h}\tilde{H}_h e^{i\varphi/h}a(x;h) = 0$$

exactly as in the case of the semiclassical Schrödinger operator above. Taking a cutoff function χ supported near y_0 and writing

$$u(y;h) = \chi(y)e^{i\varphi(y)/h}a(y;h)$$

as before, we have the same argument for exponential smallness except where we commute $\tilde{H}_h$ past the cutoff function χ. Because $\Im\varphi(y)$ increases more slowly, we only have

$$|e^{i\varphi(y)/h}| \leq e^{-1/(Ch^{1/2})}, \quad y \in \operatorname{supp}(\chi').$$

We arrive at

$$\|\tilde{H}_h u(y;h)\|_{L^2} \leq Ce^{-1/(Ch^{1/2})}$$

and

$$\|u(y;h)\|_{L^2} \geq \frac{1}{C}h^{1/8}$$

for h sufficiently small and positive. Conjugating by the change of variables $y = (\Re z)^{1/2}x$ with which we began and ignoring harmless powers of $h = (\Re z)^{-1}$ proves the theorem. □

20.9 Appendix: Spectral projections of the rotated oscillator

Asymptotics for the norms of the spectral projections of the rotated oscillator may be found using an established integral formula involving the Hermite functions, pointed out in [13], and asymptotics of the Legendre polynomials. This approach is analogous to one applied to the shifted harmonic oscillator in [51, Sec. 2], and it simplifies and sharpens the result of [27].

The eigenfunctions of H defined in (20.35) can be written explicitly through a complex scaling of Hermite functions:

$$H\left(h_k(e^{i\theta/2}x)\right) = (2k+1)h_k(e^{i\theta/2}x), \tag{20.88}$$

where h_k denote (normalized) Hermite functions. The eigenfunctions of the adjoint H^* are obtained by complex conjugation, and it is easy to verify the biorthonormal relation

$$\langle h_k(e^{i\theta/2}x), h_l(e^{-i\theta/2}x)\rangle = \delta_{kl}. \tag{20.89}$$

One may show that the eigenfunctions are complete in $L^2(\mathbb{R})$, the corresponding eigenvalues are algebraically simple, and there are no other points in the spectrum, *cf* [22]. Consequently, the spectral projections P_k of H can be written as

$$P_k = h_k(e^{i\theta/2}x)\langle h_k(e^{-i\theta/2}x), \cdot\rangle. \tag{20.90}$$

The Cauchy-Schwarz inequality, the biorthonormal relation (20.89), and symmetries of the Hermite functions can be used to show that

$$\|P_k\| = \|h_k(e^{i\theta/2}x)\|\|h_k(e^{-i\theta/2}x)\| = \|h_k(e^{i\theta/2}x)\|^2. \tag{20.91}$$

The resulting norms can be calculated explicitly. As pointed out by F. Bagarello in [13], the formula [59, Eq. 2.20.16.2, p. 502]

$$\begin{aligned}&\int_0^\infty e^{-ax^2} H_k(bx)H_k(cx)\mathrm{d}x \\ &\quad = \frac{2^{k-1}k!\sqrt{\pi}}{a^{(k+1)/2}}(b^2+c^2-a)^{k/2}\mathcal{P}_k\left(\frac{bc}{\sqrt{a(b^2+c^2-a)}}\right),\end{aligned} \tag{20.92}$$

which is valid if $\Re a > 0$ and where $\mathcal{P}_k$ are the Legendre polynomials, yields

$$\|P_k\| = \frac{1}{(\cos\theta)^{1/2}}\mathcal{P}_k\left(\frac{1}{\cos\theta}\right). \tag{20.93}$$

The final result comes from the asymptotic behaviour of $\mathcal{P}_k(x)$, *cf* the Laplace-Heine formula [76, Thm. 8.21.1] or its generalization [76, Thm. 8.21.2] which provides further terms:

$$\|P_k\| = \frac{1}{\sqrt{2\pi k|\sin\theta|}}\left(\frac{1+|\sin\theta|}{\cos\theta}\right)^{k+1/2}(1+o(1)). \tag{20.94}$$

We note that this exponential factor agrees with (20.37) and with [27], [38], following a simple computation in [79, Ex. 3.6].

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References

[1] Recall that "self-adjointness" of a densely defined operator H, *i.e.* $H = H^*$, is a much stronger property than being just "Hermitian" or "symmetric", *i.e.* $H \subset H^*$. On the other hand, the terms "non-Hermitian" and "non-self-adjoint" can be read as synonyms in the present paper, since we are concerned with a "fundamental non-self-adjointness" caused for instance by complex coefficients of differential operators; that is, we are not interested in closed symmetric non-self-adjoint operators here.

[2] Bounded and boundedly invertible Ω means $\Omega, \Omega^{-1} \in \mathscr{B}(\mathcal{H})$, where $\mathscr{B}(\mathcal{H})$ denotes the space of bounded operators on $\mathcal{H}$ to $\mathcal{H}$.

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Chapter 21

Pseudospectra of the Schrödinger operator with a discontinuous complex potential

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Pseudospectra of the Schrödinger operator with a discontinuous complex potential

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Abstract. We study spectral properties of the Schrödinger operator with an imaginary sign potential on the real line. By constructing the resolvent kernel, we show that the pseudospectra of this operator are highly non-trivial, because of a blow-up of the resolvent at infinity. Furthermore, we derive estimates on the location of eigenvalues of the operator perturbed by complex potentials. The overall analysis demonstrates striking differences with respect to the weak-coupling behaviour of the Laplacian.

Keywords: pseudospectra, non-self-adjointness, Schrdinger operators, discontinuous potential, weak coupling, Birman-Schwinger principle

MSC (2010): 34L15, 47A10, 47B44, 81Q12

21.1 Introduction

Extensive work has been done recently in understanding the spectral properties of non-self-adjoint operators through the concept of *pseudospectrum.* Referring to by now classical monographs by Trefethen and Embree [33] and Davies [8], we define the pseudospectrum of an operator T in a Hilbert space $\mathcal{H}$ to be the collection of sets

$$\sigma_\varepsilon(T) := \sigma(T) \cup \left\{ z \in \mathbb{C} : \, \|(T-z)^{-1}\| > \varepsilon^{-1} \right\} , \tag{21.1}$$

parametrised by $\varepsilon > 0$, where $\|\cdot\|$ is the operator norm of $\mathcal{H}$. If T is self-adjoint (or more generally normal), then $\sigma_\varepsilon(T)$ is just an ε-tubular neighbourhood of the spectrum $\sigma(T)$. Universally, however, the pseudospectrum is a much more reliable spectral description of T than the spectrum itself. For instance, it is the pseudospectrum that measures the instability of the spectrum under small perturbations by virtue of the formula

$$\sigma_\varepsilon(T) = \bigcup_{\|U\| \leq 1} \sigma(T + \varepsilon U) \,. \tag{21.2}$$

Leaving aside a lot of other interesting situations, let us recall the recent results when T is a differential operator. As a starting point we take the harmonic-oscillator Hamiltonian with complex frequency, which is also known as the rotated or Davies' oscillator (see [8, Sec. 14.5] for a review and references). Although the complexification has a little effect on the spectrum (the eigenvalues are just rotated in the complex plane), a careful spectral analysis reveals drastic changes in basis and other more delicate spectral properties of the operator, in particular, the spectrum is highly unstable against small perturbations, as a consequence of the pseudospectrum containing regions very far from the spectrum. Similar peculiar spectral properties have been established for complex anharmonic oscillators (to the references quoted in [8, Sec. 14.5], we add [15, 24] for the most recent results), quadratic elliptic operators [27, 17, 34], complex cubic oscillators [30, 16, 21, 26], and other models (see the recent survey [21] and references therein).

A distinctive property of the complexified harmonic oscillator is that the associated spectral problem is explicitly solvable in terms of special functions. A powerful tool to study the pseudospectrum in the situations where explicit solutions are not available is provided by microlocal analysis [7, 39, 11]. The weak point of the semiclassical methods is the usual hypothesis that the coefficients of the differential operator are smooth enough (*e.g.* the potential of the Schrödinger operator must be at least continuous), and it is indeed the case of all the models above. Another common feature of the differential operators whose pseudospectrum has been analysed so far is that their spectrum consists of discrete eigenvalues only.

The objective of the present work is to enter an unexplored area of the pseudospectral world by studying the pseudospectrum of a non-self-adjoint Schrödinger operator whose *potential is discontinuous* and, at the same time, such that the *essential spectrum is not empty.* Among various results described below, we prove that the pseudospectrum is non-trivial, despite the boundedness of the potential. Namely, we show that the norm of the resolvent can become arbitrarily large outside a fixed neighbourhood of its spectrum. We hope that our results will stimulate further analysis of non-self-adjoint differential operators with singular coefficients.

21.2 Main results

In this section we introduce our model and collect the main results of the paper. The rest of the paper is primarily devoted to proofs, but additional results can be found there, too.

21.2.1 The model

Motivated by the role of step-like potentials as toy models in quantum mechanics, in this paper we consider the Schrödinger operator in $L^2(\mathbb{R})$ defined by

$$H := -\frac{d^2}{dx^2} + i\,\mathrm{sgn}(x)\,, \qquad \mathsf{D}(H) := W^{2,2}(\mathbb{R})\,. \tag{21.3}$$

In fact, H can be considered as an infinite version of the $\mathcal{PT}$-symmetric square well introduced in [37] and further investigated in [38, 29].

Note that H is obtained as a bounded perturbation of the (self-adjoint) Hamiltonian of a free particle in quantum mechanics, which we shall simply denote here by $-\Delta$. Consequently, H is well defined (*i.e.* closed and densely defined). In fact, H is m-sectorial with the numerical range (defined, as usual, by the set of all complex numbers $(\psi, H\psi)$ such that $\psi \in \mathsf{D}(H)$ and $\|\psi\| = 1$) coinciding with the closed half-strip

$$\mathsf{Num}(H) = \overline{\mathcal{S}}\,, \qquad \text{where} \qquad \mathcal{S} := [0, +\infty) + i\,(-1, 1)\,. \tag{21.4}$$

The adjoint of H, denoted here by H^*, is simply obtained by changing $+i$ to $-i$ in (21.3). Consequently, H is neither self-adjoint nor normal. However, it is $\mathcal{T}$-self-adjoint (*i.e.* $H^* = \mathcal{T}H\mathcal{T}$), where $\mathcal{T}$ is the antilinear operator of complex conjugation (*i.e.* $\mathcal{T}\psi := \overline{\psi}$). At the same time, H is $\mathcal{P}$-self-adjoint, where $\mathcal{P}$ is the parity operator defined by $(\mathcal{P}\psi)(x) := \psi(-x)$. Finally, H is $\mathcal{PT}$-symmetric in the sense of the validity of the commutation relation $[H, \mathcal{PT}] = 0$.

Due to the analogy of the time-dependent Schrödinger equation for a quantum particle subject to an external electromagnetic field and the paraxial approximation for a monochromatic light propagation in optical media [23], the dynamics generated by (21.3) can experimentally be realised using optical systems. The physical significance of $\mathcal{PT}$-symmetry is a balance between gain and loss [5].

21.2.2 The spectrum

As a consequence of (21.4), the spectrum of H is contained in $\overline{\mathcal{S}}$. Moreover, the $\mathcal{PT}$-symmetry implies that the spectrum is symmetric with respect to the real axis. By constructing the resolvent of H and employing suitable singular sequences for H, we shall establish the following result.

Proposition 21.1. *We have*

$$\sigma(H) = \sigma_{\mathrm{ess}}(H) = [0, +\infty) + i\,\{-1, +1\}\,. \tag{21.5}$$

The fact that the two rays $[0, +\infty) \pm i$ form the essential spectrum of H is expectable, because they coincide with the spectrum of the shifted Laplacian $-\Delta \pm i$ in $L^2(\mathbb{R})$ and the essential spectrum of differential operators is known to depend on the behaviour of their coefficients at infinity only (*cf* [12, Sec. X]). The absence of spectrum outside the rays is less obvious.

In fact, the spectrum in (21.5) is purely continuous, *i.e.* $\sigma(H) = \sigma_{\mathrm{c}}(H)$, for it can be easily checked that no point from the set on the right hand side of (21.5) can be an eigenvalue of H (as well as H^*). An alternative way how to *a priori* show the absence of the residual spectrum of H, $\sigma_{\mathrm{r}}(H)$, is to employ the $\mathcal{T}$-self-adjointness of H (*cf* [20, Sec. 5.2.5.4]).

21.2.3 The pseudospectrum

Before stating the main results of this paper, let us recall that a closed operator T is said to have *trivial pseudospectra* if, for some positive constant κ, we have

$$\forall \varepsilon > 0\,, \qquad \sigma_\varepsilon(T) \subset \big\{z : \mathrm{dist}\,\big(z, \sigma(T)\big) \leq \kappa\,\varepsilon\big\}\,,$$

or equivalently,

$$\forall z \in \mathbb{C} \setminus \sigma(T)\,, \qquad \|(T - z)^{-1}\| \leq \frac{\kappa}{\mathrm{dist}\,\big(z, \sigma(T)\big)}\,. \tag{21.6}$$

Normal operators have trivial pseudospectra, because for them the equality holds in (21.6) with $\kappa = 1$.

In view of (21.4), in our case (21.6) holds with $\kappa = 1$ if the resolvent set is replaced by $\mathbb{C} \setminus \overline{\mathcal{S}}$. However, the following statement implies that (21.6) cannot hold inside the half-strip $\mathcal{S}$.

Theorem 21.1. *For all $\varepsilon > 0$, there exists a positive constant r_0 such that, for all $z \in \mathcal{S}$ with $\Re z \geq r_0$,*

$$(1-\varepsilon)\,\frac{\Re z}{\sqrt{1-(\Im z)^2}} \leq \|(H-z)^{-1}\| \leq 4\,(1+\varepsilon)\,\frac{\Re z}{1-|\Im z|}\,. \tag{21.7}$$

Although the estimates give a rather good description of the qualitative shape of the pseudospectra, the constants and dependence on $\operatorname{dist}(z,\sigma(H)) = 1-|\Im z|$ for $z \in \mathcal{S}$ are presumably not sharp.

In view of Theorem 21.1, H represents another example of a $\mathcal{PT}$-symmetric operator with non-trivial pseudospectra. The present study can be thus considered as a natural continuation of the recent works [30, 16, 21]. However, let us stress that the complex perturbation in the present model is bounded. Moreover, comparing the present setting with the situation when (21.3) is subject to an extra Dirichlet condition at zero (*cf* Section 21.7.3), the difference between these two realisations is indeed seen on the pseudospectral level only.

Even though the step-like shape of the potential in (21.3) is a feature of the present study, we stress that the discontinuity by itself is not the source of the non-trivial pseudospectra, see Remark 21.3 below.

The pseudospectrum of H computed numerically using Eigtool [36] by Mark Embree is presented in Figure 21.1.

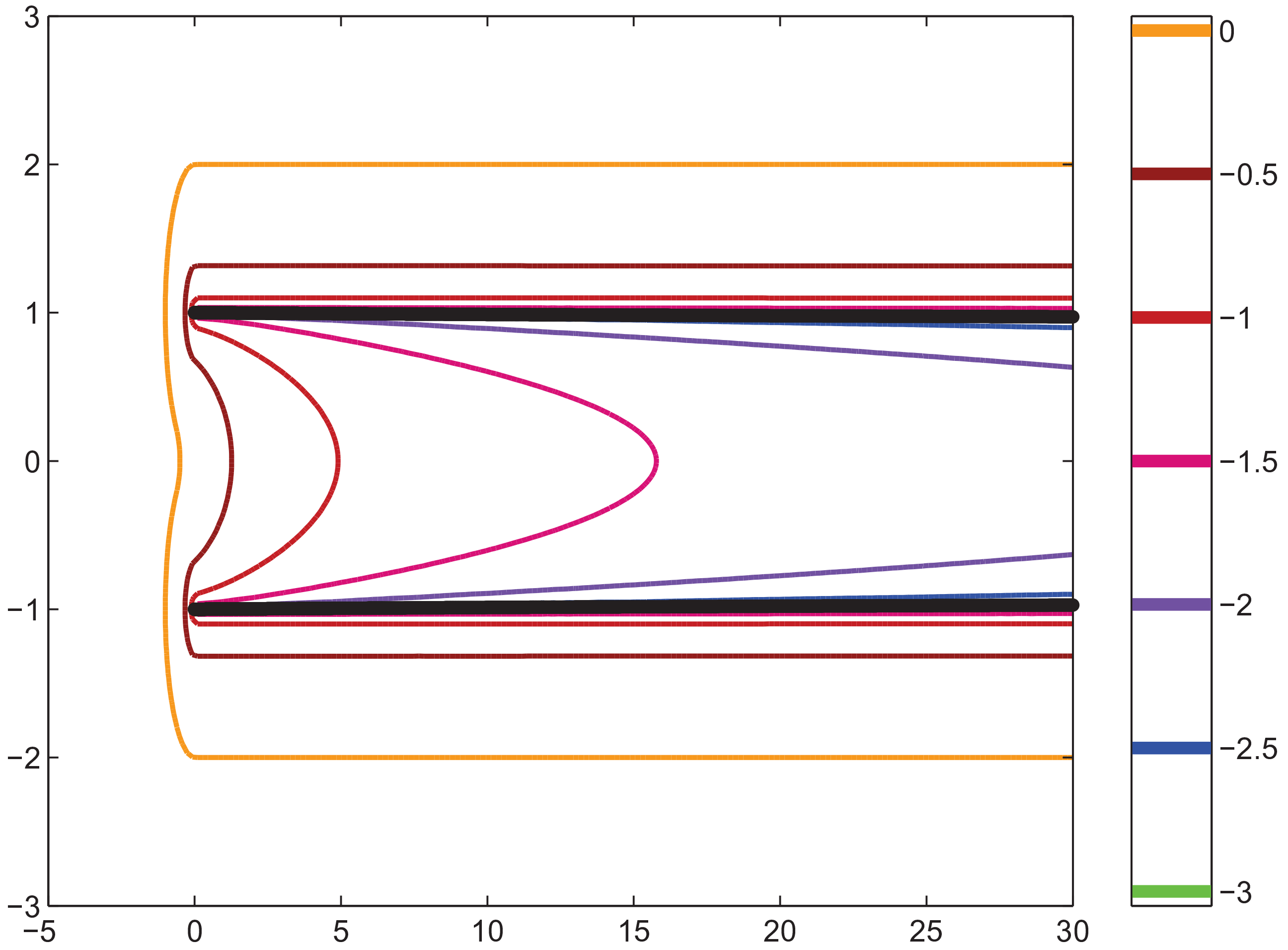

Figure 21.1: The curves $\|(H-z)^{-1}\| = \varepsilon^{-1}$ in the complex z-plane computed for several values of ε; the different colours correspond to $\log_{10}\varepsilon$, while the thick black lines are the essential spectrum of H. *(Courtesy of Mark Embree.)*

21.2.4 Weak coupling

Inspired by (21.2), we eventually consider the perturbed operator

$$H_\varepsilon := H \dot{+} \varepsilon V \tag{21.8}$$

in the limit as $\varepsilon \to 0$. Here V is the operator of multiplication by a function $V \in L^1(\mathbb{R})$ that we denote by the same letter. Since V is not necessarily relatively bounded with respect to H, the dotted sum in (21.8) is understood in the sense of forms. We remark that the perturbation does not change the essential spectrum, *i.e.*, $\sigma_{\mathrm{ess}}(H_\varepsilon) = \sigma_{\mathrm{ess}}(H)$, and recall Proposition 21.1.

If H were the free Hamiltonian $-\Delta$ and V were real-valued, the problem (21.8) with $\varepsilon \to 0$ is known as the regime of *weak coupling* in quantum mechanics. In that case, it is well known that (under some extra assumptions on V) the perturbed operator $-\Delta \dotplus \varepsilon V$ possesses a unique discrete eigenvalue for all small positive ε if, and only if, the integral of V is non-positive (see [32] for the original work). This robust existence of "weakly coupled bound states" is of course related to the singularity of the resolvent kernel of the free Hamiltonian at the bottom of the essential spectrum. Indeed, these bound states do not exist in three and higher dimensions, which is in turn related to the validity of the Hardy inequality for the free Hamiltonian (see, *e.g.*, [35]).

Complex-valued perturbations of the free Hamiltonian have been intensively studied in recent years [1, 14, 6, 22, 9, 13, 10]. In [4, 25] the authors consider perturbations of an operator which is by itself non-self-adjoint. In all of these papers, however, the results are inherited from properties of the resolvent of the free Hamiltonian.

In the present setting, the unperturbed operator H is non-self-adjoint. Moreover, its resolvent kernel has no local singularity, but it blows up as $|z| \to +\infty$ when $|\Im z| < 1$, see Section 21.3. Consequently, discrete eigenvalues of H_ε can only "emerge from the infinity", but not from any finite point of (21.5). The statement is made precise by virtue of the following result.

Theorem 21.2. *Let $V \in L^1\big(\mathbb{R}, (1+x^2)\,dx\big)$. There exists a positive constant C (independent of V and ε) such that, whenever*

$$\varepsilon \left\|(1+|\cdot|^2)V\right\|_{L^1(\mathbb{R})} \leq \frac{1}{C}\,,$$

we have

$$\sigma_{\mathrm{p}}(H_\varepsilon) \subset \overline{\mathbb{S}} \cap \left\{ \Re z \geq \frac{C}{\varepsilon^2 \, \|V\|^2_{L^1(\mathbb{R})}} \right\} . \tag{21.9}$$

It is interesting to compare this estimate on the location of possible eigenvalues of H_ε with the celebrated result of [1]

$$\sigma_{\mathrm{p}}(-\Delta \dotplus \varepsilon V) \subset \left\{ |z| \leq \frac{\varepsilon^2 \, \|V\|^2_{L^1(\mathbb{R})}}{4} \right\} . \tag{21.10}$$

Our bound (21.9) can be indeed read as an inverse of (21.10). It demonstrates how much the present situation differs from the study of weakly coupled eigenvalues of the free Hamiltonian.

Under some additional assumptions on V, the claim of Theorem 21.2 can be improved in the following way.

Theorem 21.3. *Let $n \geq 2$ and $V \in L^1\big(\mathbb{R}, (1+x^{2n})\,dx\big) \cap W^{1,1}(\mathbb{R})$. There exist positive constants ε_0 and C such that, for all $\varepsilon \in (0, \varepsilon_0)$, we have*

$$\sigma_{\mathrm{p}}(H_\varepsilon) \subset \overline{\mathbb{S}} \cap \left\{ \Re z \geq \frac{C}{\varepsilon^{2n}} \right\} . \tag{21.11}$$

In particular, if for instance V belongs to the Schwartz space $\mathscr{S}(\mathbb{R})$, then every eigenvalue $\lambda(\varepsilon)$ of H_ε must "escape to infinity" faster than any power of ε^{-1} as $\varepsilon \to 0$, namely $|\lambda(\varepsilon)|^{-1} = \mathcal{O}(\varepsilon^\infty)$.

Remark 21.1. The reader will notice that statement (21.9) differs from (21.11) in that the latter does not highlight the dependence of the right hand side on the potential V but only on its amplitude ε. The reason is that it is the behaviour of H_ε on diminishing ε that primarily interests us. Moreover, the proofs of the theorems are different and it would be cumbersome (but doable in principle) to gather the dependence of the right hand side in (21.11) on (different) norms of V.

21.2.5 The content of the paper

The organisation of this paper is as follows.

In Section 21.3, we find the integral kernel of the resolvent $(H-z)^{-1}$, *cf* Proposition 21.2, and use it to prove Proposition 21.1.

In Section 21.4, the explicit formula of the resolvent kernel is further exploited in order to prove Theorem 21.1.

The definition of the perturbed operator (21.8) and its general properties are established in Section 21.5. In particular, we locate its essential spectrum (Proposition 21.3) and prove the Birman-Schwinger principle (Theorem 21.4).

Section 21.6 is divided into two respective subsections, in which we prove Theorems 21.2 and 21.3 with help of the Birman-Schwinger principle and, again, using the explicit formula of the resolvent kernel.

Finally, in Section 21.7, we present two concrete examples of the perturbed operator (21.8). Moreover, we make a comparison of the present study with a decoupled model due to an extra Dirichlet condition.

21.3 The resolvent and spectrum

Our goal in this section is to obtain an integral representation of the resolvent of H. Using that result, we give a proof of Proposition 21.1.

In the following, we set

$$k_+(z) := \sqrt{i-z} \qquad \text{and} \qquad k_-(z) := \sqrt{-i-z}\,,$$

where we choose the principal value of the square root, *i.e.*, $z \mapsto \sqrt{z}$ is holomorphic on $\mathbb{C} \setminus (-\infty, 0]$ and positive on $(0, +\infty)$.

Proposition 21.2. *For all $z \notin \mathbb{R}_+ + i\{-1,1\}$, $H - z$ is invertible and, for every $f \in L^2(\mathbb{R})$,*

$$[(H-z)^{-1}f](x) = \int_{\mathbb{R}} \mathcal{R}_z(x,y)\, f(y)\, dy\,, \tag{21.12}$$

where

$$\mathcal{R}_z(x,y) := \begin{cases} \dfrac{1}{k_+(z)+k_-(z)}\, e^{-k_\pm(z)|x| - k_\mp(z)|y|}\,, & \pm x \geq 0\,,\ \pm y \leq 0\,, \\ \dfrac{1}{2k_\pm(z)}\, e^{-k_\pm(z)|x-y|} & \\ \qquad \pm \dfrac{k_+(z)-k_-(z)}{2k_\pm(z)\big(k_+(z)+k_-(z)\big)}\, e^{-k_\pm(z)|x+y|}\,, & \pm x \geq 0\,,\ \pm y \geq 0\,. \end{cases} \tag{21.13}$$

Remark 21.2. The kernel $\mathcal{R}_z(x,y)$ is clearly bounded for every $(x,y) \in \mathbb{R}^2$ and fixed $z \neq \pm i$. Moreover, using (21.24) below, it can be shown that it remains bounded for $z = \pm i$ as well. Hence, contrary to the case of the resolvent kernel of the free Hamiltonian $-\Delta$ in one or two dimensions, the resolvent kernel of H has *no local singularity*. On the other hand, and again contrary to the case of the Laplacian, for all fixed $(x,y) \in \mathbb{R}^2$, $|\mathcal{R}_z(x,y)| \longrightarrow +\infty$ as $\Re z \to +\infty$, $z \in \mathcal{S}$. Hence, the kernel exhibits a *blow-up at infinity*. The absence of singularity will play a fundamental role in the analysis of weakly coupled eigenvalues in Section 21.6. Moreover, we shall see in Section 21.4 that the singular behaviour at infinity is responsible for the spectral instability of H.

Proof of Proposition 21.2. Let $z \notin [0,\infty) + i\{-1,1\}$ and $f \in L^2(\mathbb{R})$. We look for the solution of the resolvent equation $(H-z)u = f$.

The general solutions $u_\pm$ of the individual equations

$$-u'' + (\pm i - z)u - f = 0 \qquad \text{in} \qquad \mathbb{R}_\pm\,, \tag{21.14}$$

where $\mathbb{R}_+ := [0, +\infty)$ and $\mathbb{R}_- := (-\infty, 0]$, are given by

$$u_\pm(x) = \alpha_\pm(x)\, e^{k_\pm(z)x} + \beta_\pm(x)\, e^{-k_\pm(z)x}\,,$$

where $\alpha_\pm$, $\beta_\pm$ are functions to be yet determined. Variation of parameters leads to the following system:

$$\begin{cases} \alpha_\pm'(x) e^{k_\pm(z)x} + \beta_\pm'(x) e^{-k_\pm(z)x} & = \ 0\,, \\ k_\pm(z)\alpha_\pm'(x) e^{k_\pm(z)x} - k_\pm(z)\beta_\pm'(x) e^{-k_\pm(z)x} & = \ -f\,. \end{cases}$$

Hence, we can choose

$$\begin{aligned} \alpha_\pm(x) &= -\frac{1}{2k_\pm(z)} \int_0^x f(y)\, e^{-k_\pm(z)y} dy + A_\pm\,, & \pm x > 0\,, \\ \beta_\pm(x) &= \frac{1}{2k_\pm(z)} \int_0^x f(y)\, e^{k_\pm(z)y} dy + B_\pm\,, & \pm x > 0\,, \end{aligned}$$

where $A_\pm, B_\pm$ are arbitray complex constants. The desired general solutions of (21.14) are then given by

$$u_\pm(x) = \frac{-1}{k_\pm(z)} \int_0^x f(y)\, \sinh\big(k_\pm(z)(x-y)\big)\, dy + A_\pm e^{k_\pm(z)x} + B_\pm e^{-k_\pm(z)x}\,, \tag{21.15}$$

with $(A_+, A_-, B_+, B_-) \in \mathbb{C}^4$.

Among these solutions, we are interested in those which satisfy the regularity conditions

$$u_+(0) = u_-(0)\,, \qquad u_+'(0) = u_-'(0)\,. \tag{21.16}$$

These conditions are equivalent to the system

$$\begin{cases} A_+ + B_+ = A_- + B_- , \\ k_+(z)A_+ - k_+(z)B_+ = k_-(z)A_- - k_-(z)B_- , \end{cases}$$

whence we obtain the following relations:

$$\begin{cases} 2A_+ = \big(k_+(z)+k_-(z)\big)A_- + \big(k_+(z)-k_-(z)\big)B_- , \\ 2B_+ = \big(k_+(z)-k_-(z)\big)A_- + \big(k_+(z)+k_-(z)\big)B_- . \end{cases} \tag{21.17}$$

Summing up, assuming (21.17), the function

$$u(x) := \begin{cases} u_+(x) & \text{if} \quad x \geq 0 , \\ u_-(x) & \text{if} \quad x \leq 0 , \end{cases} \tag{21.18}$$

belongs to $W^{2,2}_{\mathrm{loc}}(\mathbb{R})$ and solves the differential equation (21.14) in the whole $\mathbb{R}$. It remains to check some decay conditions as $x \to \pm\infty$ in addition to (21.17). This can be done by setting

$$A_+ := \frac{1}{2k_+(z)} \int_0^{+\infty} f(y)\, e^{-k_+(z)y} dy , \tag{21.19}$$

$$B_- := \frac{1}{2k_-(z)} \int_{-\infty}^{0} f(y)\, e^{k_-(z)y} dy . \tag{21.20}$$

Indeed, then

$$\begin{aligned} u_+(x) \quad = \quad & -\frac{1}{2k_+(z)}\, e^{k_+(z)x} \int_x^{+\infty} f(y)\, e^{-k_+(z)y} dy \\ & + e^{-k_+(z)x} \left(\frac{1}{2k_+(z)} \int_0^x f(y)\, e^{k_+(z)y} dy + B_+ \right) \end{aligned}$$

goes to 0 as $x \to +\infty$, and similarly for u_-.

By gathering relations (21.17), (21.19) and (21.20), we obtain the following values for A_- and B_+:

$$\begin{aligned} A_- = {} & \frac{1}{k_+(z)+k_-(z)} \int_0^{+\infty} f(y)\, e^{-k_+(z)y} dy \\ & - \frac{k_+(z)-k_-(z)}{2k_-(z)\big(k_+(z)+k_-(z)\big)} \int_{-\infty}^{0} f(y)\, e^{k_-(z)y} dy , \end{aligned} \tag{21.21}$$

$$\begin{aligned} B_+ = {} & \frac{k_+(z)-k_-(z)}{2k_+(z)\big(k_+(z)+k_-(z)\big)} \int_0^{+\infty} f(y)\, e^{-k_+(z)y} dy \\ & + \frac{1}{k_+(z)+k_-(z)} \int_{-\infty}^{0} f(y)\, e^{k_-(z)y} dy . \end{aligned} \tag{21.22}$$

Replacing the constants A_+, A_-, B_+, B_- by their values (21.19), (21.21), (21.22) and (21.20), respectively, expression (21.18) with (21.15) gives the desired integral representation

$$u(x) = \int_{\mathbb{R}} \mathcal{R}_z(x,y)\, f(y)\, dy \tag{21.23}$$

for a decaying solution of the differential equation (21.14) in $\mathbb{R}$.

To complete the proof, it remains to check that u given by (21.23) is indeed in the operator domain $\mathsf{D}(H) = W^{2,2}(\mathbb{R})$. Using for instance the Schur test (*cf* (21.28) below), it is straightforward to check that u is in $L^2(\mathbb{R})$ provided that $f \in L^2(\mathbb{R})$. Therefore $u'' = (i \operatorname{sign} x - z)u - f \in L^2(\mathbb{R})$, whence $u \in W^{2,2}(\mathbb{R})$ and $u = (H-z)^{-1} f$. □

This representation of the resolvent will be used in Sections 21.5 and 21.6 to study the location of weakly coupled eigenvalues. It will also enable us to prove the existence of non-trivial pseudospectra in Section 21.4. In this section we use it to prove Proposition 21.1.

Proof of Proposition 21.1. According to Proposition 21.2, we have

$$\sigma(H) \subset \mathbb{R}_+ + i\,\{-1, +1\} .$$

It remains to prove the inverse inclusion. This can be achieved by a standard singular sequence construction.

Let $(a_j)_{j\geq 1}$ be a real increasing sequence such that, for all $j \geq 1$, $a_{j+1} - a_j > 2j+1$. Let $\xi_j \in C_0^\infty(\mathbb{R})$ be such that Supp $\xi_j \subset (a_j - j, a_j + j)$, $\xi_j(x) = 1$ for all $x \in [a_j - 1, a_j + 1]$, and

$$\sup |\xi_j'| \leq \frac{C}{j}\,, \qquad \sup |\xi_j''| \leq \frac{C}{j^2}\,,$$

for some $C > 0$.

Then, for all $r \geq 0$, the sequence

$$u_j^\pm(x) := C_j\, \xi_j(\pm x)\, e^{irx}\,,$$

where C_j is chosen so that $\|u_j^\pm\| = 1$, is a singular sequence for H corresponding to $z = \pm i + r$ in the sense of [12, Def. IX.1.2]. Hence, according to [12, Thm. IX.1.3], we have

$$\sigma(H) \supset \mathbb{R}_+ + i\,\{-1, +1\}\,.$$

This completes the proof of the proposition. □

21.4 Pseudospectral estimates

The main purpose of this section is to give a proof of Theorem 21.1.

Proof of Theorem 21.1. Let $z = \tau + i\delta$, where $\tau > 0$ and $\delta \in (-1, 1)$. Recall our convention for the square root we fixed at the beginning of Section 21.3. The following expansions hold

$$\begin{aligned} k_+(z) &= \sqrt{i(1-\delta) - \tau} = i\sqrt{\tau - i(1-\delta)} = i\sqrt{\tau} + \frac{1-\delta}{2\sqrt{\tau}} + \mathcal{O}\left(\frac{1}{|\tau|^{3/2}}\right), \\ k_-(z) &= \sqrt{i(-1-\delta) - \tau} = -i\sqrt{\tau + i(1+\delta)} = -i\sqrt{\tau} + \frac{1+\delta}{2\sqrt{\tau}} + \mathcal{O}\left(\frac{1}{|\tau|^{3/2}}\right), \end{aligned} \tag{21.24}$$

as $\tau \to +\infty$. As a consequence, we have the asymptotics

$$|k_+(z)| \sim \sqrt{\tau}\,, \qquad |k_-(z)| \sim \sqrt{\tau}\,, \tag{21.25}$$

$$\Re k_+(z) \sim \frac{1-\delta}{2\sqrt{\tau}}\,, \qquad \Re k_-(z) \sim \frac{1+\delta}{2\sqrt{\tau}}\,, \tag{21.26}$$

$$|k_+(z) + k_-(z)| \sim \frac{1}{\sqrt{\tau}}\,, \qquad |k_+(z) - k_-(z)| \sim 2\sqrt{\tau}\,, \tag{21.27}$$

as $\tau \to +\infty$.

Let us prove the upper bound in (21.7) using the Schur test:

$$\|(H-z)^{-1}\|^2 \;\leq\; \sup_{x\in\mathbb{R}} \int_{\mathbb{R}} |\mathcal{R}_z(x,y)|\, dy \;\cdot\; \sup_{y\in\mathbb{R}} \int_{\mathbb{R}} |\mathcal{R}_z(x,y)|\, dx\,. \tag{21.28}$$

After noticing the symmetry relation $\mathcal{R}_z(x,y) = \mathcal{R}_z(y,x)$ valid for all $(x,y) \in \mathbb{R}^2$ (which is a consequence of the $\mathcal{T}$-self-adjointness of H), we simply have

$$\|(H-z)^{-1}\| \;\leq\; \sup_{x\in\mathbb{R}} \int_{\mathbb{R}} |\mathcal{R}_z(x,y)|\, dy\,. \tag{21.29}$$

By virtue of (21.13), for all $x > 0$,

$$\begin{aligned} \int_{\mathbb{R}} |\mathcal{R}_z(x,y)|\, dy \;&\leq\; \frac{1}{|k_+(z) + k_-(z)|} \int_{-\infty}^{0} e^{-\Re k_+(z)\, x + \Re k_-(z)\, y}\, dy \\ &\quad + \frac{1}{2|k_+(z)|} \int_0^{+\infty} e^{-\Re k_+ |x-y|}\, dy \\ &\quad + \frac{|k_+(z) - k_-(z)|}{2|k_+(z)||k_+(z) + k_-(z)|} \int_0^{+\infty} e^{-\Re k_+(z)(x+y)}\, dy \\ &\leq \frac{1}{\Re k_-(z) |k_+(z) + k_-(z)|} + \frac{1}{2\Re k_+(z) |k_+(z)|} \\ &\quad + \frac{|k_+(z) - k_-(z)|}{2\Re k_+(z)|k_+(z)||k_+(z) + k_-(z)|}\,. \end{aligned} \tag{21.30}$$

Similarly, if $x < 0$,

$$\int_{\mathbb{R}} |\mathcal{R}_z(x,y)|\,dy \;\le\; \frac{1}{\Re k_+(z)|k_+(z)+k_-(z)|} + \frac{1}{2\Re k_-(z)|k_-(z)|} + \frac{|k_+(z)-k_-(z)|}{2\Re k_-(z)|k_-(z)||k_+(z)+k_-(z)|}\,. \tag{21.31}$$

According to (21.25)–(21.27), the right hand sides in (21.30) and (21.31) are both equivalent to

$$2\tau\big[(1+\delta)^{-1} + (1-\delta)^{-1}\big] \le \frac{4\tau}{1-|\delta|}\,,$$

whence (21.29) yields the upper bound in (21.7).

In order to get the lower bound, we set

$$f_0(x) := e^{-\overline{k_+(z)}\,x}\chi_{(0,\infty)}(x)\,, \tag{21.32}$$

where χ_Σ denotes the characteristic function of a set Σ. Then according to (21.13),

$$\|(H-z)^{-1}f_0\|^2 \ge \int_{-\infty}^{0}\left|\frac{1}{k_+(z)+k_-(z)}\int_0^{+\infty} e^{k_-(z)\,x - 2\Re k_+(z)\,y}\,dy\right|^2 dx \tag{21.33}$$

$$= \frac{1}{|k_+(z)+k_-(z)|^2}\int_{-\infty}^{0} e^{2\Re k_-(z)\,x}\,dx\left(\int_0^{+\infty} e^{-2\Re k_+(z)\,y}\,dy\right)^2 \tag{21.34}$$

$$= \frac{1}{\big(2\Re k_+(z)\big)^2\,2\Re k_-(z)\,|k_+(z)+k_-(z)|^2}\,. \tag{21.35}$$

On the other hand, we have

$$\|f_0\|^2 = \frac{1}{2\Re k_+(z)}\,. \tag{21.36}$$

Hence, using (21.26) and (21.27),

$$\frac{\|(H-z)^{-1}f_0\|}{\|f_0\|} \ge \frac{1}{2\sqrt{\Re k_+(z)\Re k_-(z)}\,|k_+(z)+k_-(z)|} \sim \frac{\tau}{\sqrt{1-\delta^2}}$$

as $\tau \to +\infty$, and the lower bound in (21.7) follows. ☐

Remark 21.3 (Irrelevance of discontinuity)**.** Although the proof above relies on the particular form of the potential $i\,\mathrm{sgn}(x)$, it turns out that the discontinuity at $x = 0$ is not responsible for the spectral instability highlighted by Theorem 21.1. Indeed, consider instead of the potential $i\,\mathrm{sgn}(x)$ a smooth potential $V(x)$ such that, for some $a > 0$, the difference

$$h(x) := i\,\mathrm{sgn}(x) - V(x)$$

is supported in the interval $[-a, 0]$. In order to get a lower bound for the norm of the resolvent of the regularised operator $\tilde{H} := -\frac{d^2}{dx^2} + V(x)$, we shall use the pseudomode

$$g_0 := (H-z)^{-1}f_0\,,$$

where the function f_0 is introduced in (21.32). Using again the asymptotic expansions (21.24), one can check that, provided that $\Re z$ is large enough,

$$\|hg_0\|^2 \le C\,(\Re z)^2$$

for some $C > 0$ independent of z. Thus, in view of (21.36), we have

$$\|(\tilde{H}-z)g_0\| \le \|f_0\| + \|hg_0\| = \mathcal{O}(\Re z)$$

as $\Re z \to +\infty$, $z \in \mathcal{S}$. On the other hand, (21.35) yields

$$\|g_0\|^2 \ge C'\,(\Re z)^{5/2}$$

for some $C' > 0$ independent of z. Consequently, g_0 is a $(\Re z)^{-1/4}$-pseudomode for $\tilde{H} - z$, or more specifically,

$$\|(\tilde{H}-z)^{-1}\| \ge c\,(\Re z)^{1/4} \tag{21.37}$$

with $c > 0$ independent of z, as $\Re z \to +\infty$, $z \in \mathcal{S}$.

Summing up, despite of the fact that the lower bound in (21.37) is not as good as that of Theorem 21.1, the presence of non-trivial pseudospectra for the operator $\tilde{H}$ clearly indicates that the discontinuity of the potential $i\,\mathrm{sgn}(x)$ does not really play any essential role in the spectral instability of H.

21.5 General properties of the perturbed operator

In this section, we state some basic properties about the perturbed operator H_ε introduced in (21.8). Here ε is not necessarily small and positive.

21.5.1 Definition of the perturbed operator

The unperturbed operator H introduced in (21.3) is associated (in the sense of the representation theorem [18, Thm. VI.2.1]) with the sesquilinear form

$$\begin{aligned} h(\psi,\phi) &:= \int_{\mathbb{R}} \psi'(x)\bar{\phi}'(x)\,dx + i\int_0^{+\infty} \psi(x)\bar{\phi}(x)\,dx - i\int_{-\infty}^0 \psi(x)\bar{\phi}(x)\,dx\,, \\ \mathsf{D}(h) &:= W^{1,2}(\mathbb{R})\,. \end{aligned}$$

In view of (21.4), h is sectorial with vertex -1 and semi-angle $\pi/4$. In fact, h is obtained as a bounded perturbation of the non-negative form q associated with the free Hamiltonian $-\Delta$,

$$\begin{aligned} q(\psi,\phi) &:= \int_{\mathbb{R}} \psi'(x)\bar{\phi}'(x)\,dx\,, \\ \mathsf{D}(q) &:= W^{1,2}(\mathbb{R})\,. \end{aligned}$$

Given any function $V \in L^1(\mathbb{R})$, let v be the sesquilinear form of the corresponding multiplication operator (that we also denote by V), *i.e.*,

$$\begin{aligned} v(\psi,\phi) &:= \int_{\mathbb{R}} V(x)\psi(x)\bar{\phi}(x)\,dx\,, \\ \mathsf{D}(v) &:= \left\{\psi \in L^2(\mathbb{R}):\ |V|^{1/2}\psi \in L^2(\mathbb{R})\right\}\,. \end{aligned}$$

As usual, we denote by $v[\psi] := v(\psi,\psi)$ the corresponding quadratic form.

Lemma 21.1. *Let $V \in L^1(\mathbb{R})$. Then $\mathsf{D}(v) \supset W^{1,2}(\mathbb{R})$ and, for every $\psi \in W^{1,2}(\mathbb{R})$,*

$$|v[\psi]| \le 2\|V\|_{L^1(\mathbb{R})}\|\psi'\|\|\psi\|\,. \tag{21.38}$$

Proof. Set $f(x) := \int_{-\infty}^x V(\xi)d\xi$. For every $\psi \in C_0^\infty(\mathbb{R})$, an integration by parts together with the Schwarz inequality yields

$$\begin{aligned} |v[\psi]| &= \left|\int_{\mathbb{R}} f'(x)|\psi(x)|^2\,dx\right| = \left|\int_{\mathbb{R}} f(x)\,2\Re\big(\psi'(x)\bar{\psi}(x)\big)\,dx\right| \\ &\le 2\|V\|_{L^1(\mathbb{R})}\|\psi'\|\|\psi\|\,. \end{aligned}$$

By density of $C_0^\infty(\mathbb{R})$ in $W^{1,2}(\mathbb{R})$, the inequality extends to all $\psi \in W^{1,2}(\mathbb{R})$ and, in particular, $|v[\psi]| < \infty$ whenever $\psi \in W^{1,2}(\mathbb{R})$. □

It follows from the lemma that v is $\frac{1}{2}$-subordinated to q, which in particular implies that v is relatively bounded with respect to q with the relative bound equal to zero. Classical stability results (see, *e.g.*, [20, Sec. 5.3.4]) then ensure that the form $q+v$ is sectorial and closed. Since h is a bounded perturbation of q, we also know that $h_1 := h+v$ is sectorial and closed. We define H_1 to be the m-sectorial operator associated with the form h_1. The representation theorem yields

$$\begin{aligned} H_1\psi &= -\psi'' + i\,\mathrm{sgn}\,\psi + V\psi\,, \\ \mathsf{D}(H_1) &= \left\{\psi \in W^{1,2}(\mathbb{R}):\ \exists\eta \in L^2(\mathbb{R}),\ \forall\phi \in W^{1,2}(\mathbb{R}),\ h_1(\psi,\phi) = (\eta,\phi)\right\} \\ &= \left\{\psi \in W^{1,2}(\mathbb{R}):\ -\psi'' + V\psi \in L^2(\mathbb{R})\right\}\,, \end{aligned} \tag{21.39}$$

where $-\psi'' + V\psi$ should be understood as a distribution. By the replacement $V \mapsto \varepsilon V$, we introduce in the same way as above the form $h_\varepsilon := h + \varepsilon v$ and the associated operator H_ε for any $\varepsilon \in \mathbb{R}$. Of course, we have $H_0 = H$.

21.5.2 The Birman-Schwinger principle

As regards spectral theory, H_ε represents a singular perturbation of H, for we are perturbing an operator with purely essential spectrum. An efficient way to deal with such problems in self-adjoint settings is the method of the *Birman-Schwinger principle*, due to which a study of discrete eigenvalues of the differential operator H_ε is transferred to a spectral analysis of an integral operator. We refer to [2, 28] for the original works and to [31, 32, 3, 19] for an extensive development of the method for Schrödinger operators. In recent years, the technique has been also applied to Schrödinger operators with complex potentials (see, *e.g.*, [1, 22, 13]). However, our setting differs from all the previous works in that the unperturbed operator H is already non-self-adjoint and its resolvent kernel substantially differs from the resolvent of the free Hamiltonian. The objective of this subsection is to carefully establish the Birman-Schwinger principle in our unconventional situation.

In the following, given $V \in L^1(\mathbb{R})$, we denote

$$V_{1/2}(x) := |V|^{1/2} e^{i \arg V(x)},$$

so that $V = |V|^{1/2} V_{1/2}$.

We have introduced H as an unbounded operator with domain $\mathsf{D}(H) = W^{2,2}(\mathbb{R})$ acting in the Hilbert space $L^2(\mathbb{R})$. It can be regarded as a bounded operator from $W^{2,2}(\mathbb{R})$ to $L^2(\mathbb{R})$. More interestingly, using the variational formulation, H can be also viewed as a bounded operator from $W^{1,2}(\mathbb{R})$ to $W^{-1,2}(\mathbb{R})$, by defining $H\psi$ for all $\psi \in W^{1,2}(\mathbb{R})$ by

$$\forall \phi \in W^{1,2}(\mathbb{R}), \qquad {}_{-1}\langle H\psi, \phi\rangle_{+1} := h(\psi, \phi),$$

where ${}_{-1}\langle \cdot, \cdot\rangle_{+1}$ denotes the duality bracket between $W^{-1,2}(\mathbb{R})$ and $W^{1,2}(\mathbb{R})$.

Similarly, in addition to regarding the multiplication operators $|V|^{1/2}$ and $V_{1/2}$ as operators from $W^{1,2}(\mathbb{R})$ to $L^2(\mathbb{R})$, we can view them as operators from $L^2(\mathbb{R})$ to $W^{-1,2}(\mathbb{R})$, due to the relative boundedness of v with respect to q (*cf* Lemma 21.1 and the text below it).

Finally, let us notice that, for all $z \in \mathbb{C} \setminus \sigma(H)$, the resolvent $(H - z)^{-1}$ can be viewed as an operator from $W^{-1,2}(\mathbb{R})$ to $W^{1,2}(\mathbb{R})$. Indeed, for all $\eta \in W^{-1,2}(\mathbb{R})$, there exists a unique $\psi \in W^{1,2}(\mathbb{R})$ such that

$$\forall \phi \in W^{1,2}(\mathbb{R}), \qquad {}_{-1}\langle \eta, \phi\rangle_{+1} = h(\psi, \phi) - z(\psi, \phi), \tag{21.40}$$

where $(\cdot, \cdot)$ denotes the inner product in $L^2(\mathbb{R})$. Hence the operator $(H - z) : W^{1,2}(\mathbb{R}) \to W^{-1,2}(\mathbb{R})$ is bijective.

With the above identifications, for all $z \in \mathbb{C} \setminus \sigma(H)$, we introduce

$$K_z := |V|^{1/2}(H - z)^{-1} V_{1/2} \tag{21.41}$$

as a bounded operator on $L^2(\mathbb{R})$ to $L^2(\mathbb{R})$. K_z is an integral operator with kernel

$$\mathcal{K}_z(x, y) := |V|^{1/2}(x)\, \mathcal{R}_z(x, y)\, V_{1/2}(y), \tag{21.42}$$

where $\mathcal{R}_z$ is the kernel of the resolvent $(H - z)^{-1}$ written down explicitly in (21.13). The following result shows that K_z is in fact compact.

Lemma 21.2. *Let $V \in L^1(\mathbb{R})$. For all $z \in \mathbb{C} \setminus \sigma(H)$, K_z is a Hilbert-Schmidt operator.*

Proof. By definition of the Hilbert-Schmidt norm,

$$\begin{aligned} \|K_z\|_{\mathrm{HS}} &= \int_{\mathbb{R}^2} |V(x)| |\mathcal{R}_z(x, y)|^2 |V(y)| \, dx \, dy \\ &\le \|V\|^2_{L^1(\mathbb{R})} \sup_{(x,y)\in\mathbb{R}^2} |\mathcal{R}_z(x, y)|^2 . \end{aligned} \tag{21.43}$$

According to (21.13), we have

$$\begin{aligned} &\sup_{(x,y)\in\mathbb{R}^2} |\mathcal{R}_z(x, y)|^2 \\ &\quad \le \frac{1}{|k_+(z) + k_-(z)|^2} + \left(\frac{1}{|k_+(z)|^2} + \frac{1}{|k_-(z)|^2} \right) \left(1 + \frac{|k_+(z) - k_-(z)|^2}{|k_+(z) + k_-(z)|^2} \right), \end{aligned}$$

where the right hand side is finite for all $z \in \mathbb{C} \setminus \sigma(H)$. □

We are now in a position to state the Birman-Schwinger principle for our operator H_ε.

Theorem 21.4 (Birman-Schwinger principle)**.** *Let $V \in L^1(\mathbb{R})$ and $\varepsilon \in \mathbb{R}$. For all $z \in \mathbb{C} \setminus \sigma(H)$, we have*

$$z \in \sigma_{\mathrm{p}}(H_\varepsilon) \quad \Longleftrightarrow \quad -1 \in \sigma(\varepsilon K_z).$$

Proof. Clearly, it is enough to establish the equivalence for $\varepsilon = 1$.

If $z \in \sigma_{\mathrm{p}}(H_1)$, then there exists a non-trivial function $\psi \in \mathsf{D}(H_1)$ such that $H_1\psi = z\psi$. In particular, $\psi \in \mathsf{D}(h_1) = W^{1,2}(\mathbb{R})$ and

$$h_1(\psi,\phi) \equiv h(\psi,\phi) + v(\psi,\phi) = z(\psi,\phi) \tag{21.44}$$

holds for every $\phi \in W^{1,2}(\mathbb{R})$. We set $g := |V|^{1/2}\psi \in L^2(\mathbb{R})$. Given an arbitrary test function $\varphi \in L^2(\mathbb{R})$, we introduce an auxiliary function $\eta := (H^* - \bar{z})^{-1}|V|^{1/2}\varphi \in W^{1,2}(\mathbb{R})$. (Note that $\sigma(H^*) = \sigma(H)$ and that the spectrum is symmetric with respect to the real axis, so the resolvent $(H^* - \bar{z})^{-1}$ is well defined. Moreover, recall that H is $\mathfrak{T}$-self-adjoint.) We have

$$\begin{aligned}
(K_z g,\varphi) &= v(\psi,\eta)\\
&= -h(\psi,\eta) + z(\psi,\eta) = \overline{-h^*(\eta,\psi) + \bar{z}(\eta,\psi)}\\
&= -\overline{{}_{-1}\langle |V|^{1/2}\varphi,\psi\rangle_{+1}}\\
&= -\overline{(\varphi,|V|^{1/2}\psi)}\\
&= -(g,\varphi)\,.
\end{aligned}$$

Here the first equality uses the integral representation (21.42) of K_z, the second equality is due to (21.44) and the equality on the third line is a version of (21.40) for H^*. Hence, g is an eigenfunction of K_z corresponding to the eigenvalue -1.

Conversely, if $-1 \in \sigma(K_z)$, then -1 is an eigenvalue of K_z, because K_z is compact (*cf* Lemma 21.2). Hence, there exists a non-trivial $g \in L^2(\mathbb{R})$ such that $K_z g = -g$. Defining, $\psi := (H - z)^{-1}V_{1/2}\, g \in W^{1,2}(\mathbb{R})$, we have

$$\begin{aligned}
h_1(\psi,\phi) &= h(\psi,\phi) - z(\psi,\phi) + z(\psi,\phi) + v(\psi,\phi)\\
&= {}_{-1}\langle V_{1/2}\, g,\psi\rangle_{+1} + z(\psi,\phi) + {}_{-1}\langle V\psi,\phi\rangle_{+1}\\
&= {}_{-1}\langle V_{1/2}\, g,\psi\rangle_{+1} + z(\psi,\phi) + {}_{-1}\langle V_{1/2}K_z g,\phi\rangle_{+1}\\
&= z(\psi,\phi)
\end{aligned}$$

for all $\phi \in W^{1,2}(\mathbb{R})$, where the eigenvalue equation is used in the last equality. It follows that $\psi \in \mathsf{D}(H)$ (*cf* (21.39)) and $H\psi = z\psi$. □

21.5.3 Stability of the essential spectrum

As the last result of this section, we locate the essential spectrum of the perturbed operator H_ε.

Since there exist various definitions of the essential spectrum for non-self-adjoint operators (*cf* [12, Sec. IX] or [20, Sec. 5.4]), we note that we use the widest (that due to Browder) in this paper. More specifically, given a closed operator T in a Hilbert space $\mathcal{H}$, we set $\sigma_{\mathrm{ess}}(T) := \sigma(T) \setminus \sigma_{\mathrm{disc}}(T)$, where the discrete spectrum is defined as the set of isolated eigenvalues λ of T which have finite algebraic multiplicity and such that $\mathsf{R}(T-\lambda)$ is closed in $\mathcal{H}$.

Our stability result will follow from the following compactness property.

Lemma 21.3. *Let $V \in L^1(\mathbb{R})$ and $\varepsilon \in \mathbb{R}$. For all $z \in \mathbb{C} \setminus [\sigma(H) \cup \sigma(H_\varepsilon)]$, the resolvent difference $(H_\varepsilon - z)^{-1} - (H - z)^{-1}$ is a compact operator in $L^2(\mathbb{R})$.*

Proof. It is straightforward to verify the resolvent equation

$$(H_\varepsilon - z)^{-1} - (H - z)^{-1} = -\varepsilon A^* B\,,$$

where

$$A := \overline{V}_{1/2}(H_\varepsilon^* - \bar{z})^{-1} \qquad \text{and} \qquad B := |V|^{1/2}(H - z)^{-1}$$

are bounded operators (recall that $\mathsf{D}(h_\varepsilon) = W^{1,2}(\mathbb{R}) \subset \mathsf{D}(v)$). It is thus enough to show that B is compact. It is equivalent to proving that BB^* is compact. However, BB^* is an integral operator with kernel

$$|V|^{1/2}(x)\,\mathcal{N}_z(x,y)\,|V|^{1/2}(y)\,,$$

where

$$\mathcal{N}_z(x,y) := \int_{\mathbb{R}} \mathcal{R}_z(x,\xi)\,\overline{\mathcal{R}_z(y,\xi)}\,d\xi$$

is the integral kernel of $(H - z)^{-1}(H^* - \bar{z})^{-1}$. Consequently,

$$\|BB^*\|_{\mathrm{HS}} \le \|V\|_{L^1(\mathbb{R})} \sup_{(x,y)\in\mathbb{R}^2} |\mathcal{N}_z(x,y)|\,. \tag{21.45}$$

Using (21.13), it is straightforward to check that, for all $z \in \mathbb{C} \setminus \sigma(H)$, $\mathcal{R}_z \in L^\infty\big(\mathbb{R}; L^2(\mathbb{R})\big)$, and thus the supremum on the right-hand side of (21.45) is a finite (z-dependent) constant. Summing up, BB^* is Hilbert-Schmidt, in particular it is compact. $\square$

Proposition 21.3. *Let $V \in L^1(\mathbb{R})$. For all $\varepsilon \in \mathbb{R}$, we have*

$$\sigma_{\mathrm{ess}}(H_\varepsilon) = \sigma_{\mathrm{ess}}(H) = \mathbb{R}_+ + i\,\{-1,+1\}\,. \tag{21.46}$$

Proof. First of all, notice that, since H_ε is m-sectorial for all $\varepsilon \in \mathbb{R}$, the intersection of the resolvent sets of H_ε and H is not empty. By Lemma 21.3 and a classical stability result about the invariance of the essential spectra under perturbations (see, *e.g.*, [12, Thm. IX.2.4]), we immediately obtain (21.46) for more restrictive definitions of the essential spectrum. To deduce the result for our definition of the essential spectrum, it is enough to notice that the exterior of $\sigma_{\mathrm{ess}}(H)$ is connected (*cf* [20, Prop. 5.4.4]). $\square$

Remark 21.4. In view of Proposition 21.3, the equivalence of Theorem 21.4 remains to hold if $\sigma_{\mathrm{p}}(H_\varepsilon)$ is replaced by $\sigma(H_\varepsilon)$ or $\sigma_{\mathrm{disc}}(H_\varepsilon)$.

21.6 Eigenvalue estimates

In this section, we consecutively prove Theorems 21.2 and 21.3.

21.6.1 Proof of Theorem 21.2

Our strategy is based on Theorem 21.4 and on estimating the norm of the Birman-Schwinger operator K_z by its Hilbert-Schmidt norm. To get a better estimate than that of (21.43), we proceed as follows.

Let us partition the complex plane into several regions where $z \mapsto \mathcal{R}_z$ has a different behaviour. We set

$$\begin{aligned} D_+ &:= \big\{z \in \mathbb{C} : \, |z-i| \le 3/2\big\} \setminus \big(\mathbb{R}_+ + i\big)\,, \\ D_- &:= \big\{z \in \mathbb{C} : \, |z+i| \le 3/2\big\} \setminus \big(\mathbb{R}_+ - i\big)\,, \\ U &:= \mathbb{C} \setminus \big(\bar{\mathcal{S}} \cup D_+ \cup D_-\big)\,, \\ W &:= \mathcal{S} \setminus \big(D_+ \cup D_-\big)\,, \end{aligned}$$

where $\mathcal{S}$ is defined in (21.4), see Figure 21.2. We have indeed

$$\mathbb{C} \setminus \big(\mathbb{R}_+ + i\{-1,1\}\big) = D_+ \cup D_- \cup U \cup W\,.$$

First, let us estimate $\sup_{\mathbb{R}^2} |\mathcal{R}_z|$ for $z \in D_+$. As $z \to i$, we have $k_+(z) \to 0$ and $k_-(z) \to \sqrt{-2i}$. Thus, there exist positive constants c_0 , c_1 and c_2 such that, for all $z \in D_+$,

$$|k_+(z) + k_-(z)| \ge \frac{1}{c_0}\,, \qquad |k_+(z) - k_-(z)| \le c_1\,, \qquad |k_-(z)| \ge \frac{1}{c_2}\,. \tag{21.47}$$

According to (21.13), we then have, for all $(x,y) \in \mathbb{R}^2$ such that $xy \le 0$,

$$|\mathcal{R}_z(x,y)| \le \frac{1}{|k_+(z) + k_-(z)|} \le c_0\,, \tag{21.48}$$

and, for all $(x,y) \in \big\{x \le 0, y \le 0\big\}$,

$$|\mathcal{R}_z(x,y)| \le \frac{1}{2|k_-(z)|}\left(1 + \frac{|k_+(z) - k_-(z)|}{|k_+(z) + k_-(z)|}\right) \le \frac{c_2}{2}(1 + c_0 c_1)\,. \tag{21.49}$$

It remains to check that there is no singularity as $z \to i$ for $x > 0$, $y > 0$:

$$\begin{aligned} |\mathcal{R}_z(x,y)| &= \frac{1}{2|k_+(z)|}\left|e^{-k_+(z)|x-y|} + \Big(-1 + \frac{2k_+(z)}{k_+(z)+k_-(z)}\Big)e^{-k_+(z)(|x|+|y|)}\right| \\ &\le \frac{1}{2|k_+(z)|}\left|e^{-k_+(z)|x-y|} - e^{-k_+(z)(|x|+|y|)}\right| + \frac{1}{|k_+(z)+k_-(z)|} \\ &\le c_0 + \frac{1}{2|k_+(z)|}\left|\Big(e^{-k_+(z)|x-y|} - 1\Big) - \Big(e^{-k_+(z)(|x|+|y|)} - 1\Big)\right| \\ &\le c_0 + \frac{|x-y| + |x| + |y|}{2} \\ &\le c_0 + |x| + |y|\,, \end{aligned} \tag{21.50}$$

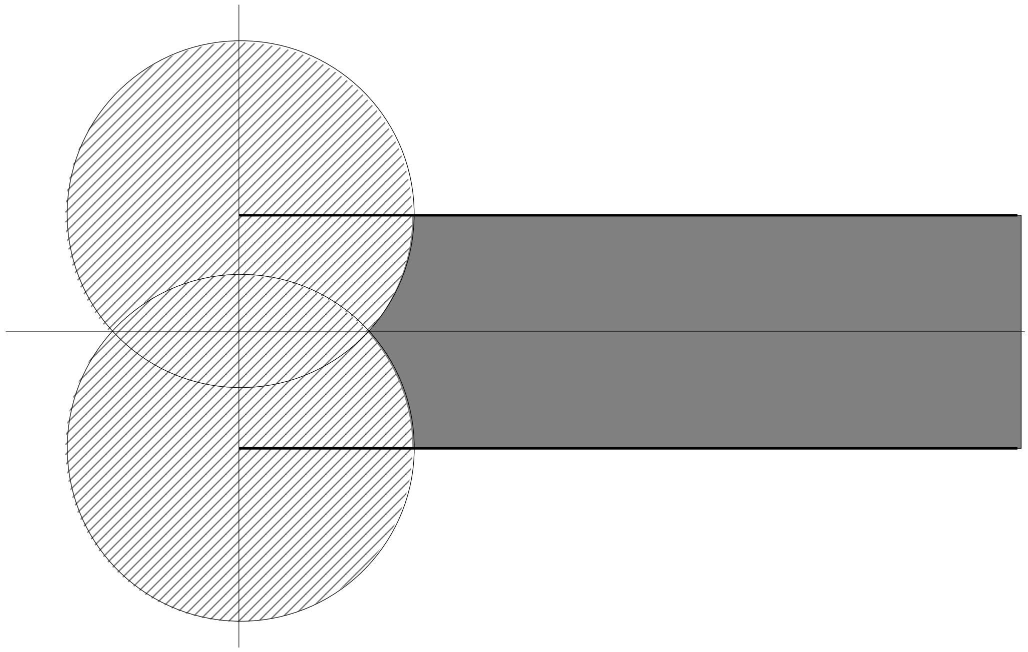

Figure 21.2: The subdomains D_+, D_-, U and W.

where we have used the inequality $|e^{-\omega} - 1| \le |\omega|$ for $\Re\omega \ge 0$. Using (21.48), (21.49) and (21.50), we then get, for all $z \in D_+$,

$$\begin{aligned}\|K_z\|_{\mathrm{HS}}^2 &\le \int_{\mathbb{R}^2} |V(x)|\Big(3c_0^2 + \frac{c_2^2}{4}(1+c_0c_1)^2 + 2\big(|x|+|y|\big)^2\Big)|V(y)|\,dx\,dy \\ &\le C_+ \left(\int_{\mathbb{R}} (1+|x|^2)|V(x)|\,dx\right)^2, \end{aligned} \tag{21.51}$$

with some $C_+ > 0$.

Similarly, one can check that there exists $C_- > 0$ such that, for all $z \in D_-$,

$$\|K_z\|_{\mathrm{HS}}^2 \le C_- \left(\int_{\mathbb{R}} (1+|x|^2)|V(x)|\,dx\right)^2 . \tag{21.52}$$

Now let us consider the region U. Notice that, as $|z| \to +\infty$, $z \in U$, we have

$$k_+(z) - k_-(z) \longrightarrow 0 \qquad \text{and} \qquad k_+(z) \sim k_-(z) \sim \sqrt{-z}\,,$$

hence $|k_+ + k_-|^{-1}$, $|k_+|^{-1}$, $|k_-|^{-1}$ and $|k_+ - k_-|$ are uniformly bounded in U. Thus, there exists $C_1 > 0$ such that, for all $z \in U$,

$$\|K_z\|_{\mathrm{HS}}^2 \le \|V\|_{L^1(\mathbb{R})}^2 \sup_{(x,y)\in\mathbb{R}^2} |\mathcal{R}_z(x,y)|^2 \le C_1 \|V\|_{L^1(\mathbb{R})}^2 . \tag{21.53}$$

Finally, for $z \in W$, we use the asymptotic expansions (21.25) and (21.27). In particular, there exist $c_3 > 0$, $c_4 > 0$ and $c_5 > 0$ such that, for all $z \in W$,

$$2|k_\pm(z)| \ge \frac{\sqrt{\Re z}}{c_3}, \quad |k_-(z) - k_+(z)| \le c_4\sqrt{\Re z}, \quad |k_+(z) + k_-(z)| \ge \frac{1}{c_5\sqrt{\Re z}} .$$

Thus, according to (21.13), we have

$$\sup_{(x,y)\in\mathbb{R}^2} |\mathcal{R}_z(x,y)| \le \frac{c_3}{\sqrt{\Re z}} + c_3c_4c_5\sqrt{\Re z} \le \sqrt{C_2 \Re z}$$

for some $C_2 > 0$, hence

$$\|K_z\|_{\mathrm{HS}}^2 \le C_2\, \Re z\, \|V\|_{L^1(\mathbb{R})}^2 . \tag{21.54}$$

Gathering (21.51), (21.52), (21.53) and (21.54), we obtain, for all $z \in \mathbb{C} \setminus \big(\mathbb{R}_+ + i\{-1, +1\}\big)$,

$$\|K_z\|_{\mathrm{HS}}^2 \le \max\Big(\max(C_+, C_-, C_1)\big\|(1+|\cdot|^2)V\big\|_{L^1(\mathbb{R})}^2, C_2\,\Re z\,\|V\|_{L^1(\mathbb{R})}^2\Big), \tag{21.55}$$

and more precisely when $z \notin \mathcal{S}$,

$$\|K_z\|_{\mathrm{HS}}^2 \le \max(C_+, C_-, C_1)\big\|(1+|\cdot|^2)V\big\|_{L^1(\mathbb{R})}^2 .$$

In particular, if $\|(1+|\cdot|^2)V\|_{L^1(\mathbb{R})}^2 < \max(C_+, C_-, C_1)^{-1}$ and either $z \notin \mathcal{S}$ or $\Re z < (C_2\,\|V\|_{L^1(\mathbb{R})}^2)^{-1}$, then $\|K_z\|_{\mathrm{HS}} < 1$ and -1 cannot be in the spectrum of K_z. After the replacement $V \mapsto \varepsilon V$, we therefore get Theorem 21.2 as a consequence of Theorem 21.4. □

21.6.2 Proof of Theorem 21.3

Let V satisfy the assumptions of Theorem 21.3 with $n \ge 2$ and $\varepsilon > 0$. The present proof is again based on Theorem 21.4, but we use a more sophisticated estimate of the norm of K_z for which the extra regularity hypotheses are needed.

The first step in our proof is to isolate the singular part of the kernel $\mathcal{K}_z$. The idea comes back to [32], where the singularity of the free resolvent $(-\Delta - z)^{-1}$ at $z = 0$ is singled out. In the present setting, however, the resolvent $(H - z)^{-1}$ is rather singular as $\Re z \to +\infty$. In other words, we want to find a decomposition of the form

$$K_z = L_z + M_z\,, \tag{21.56}$$

where $\|L_z\| \to +\infty$ as $\Re z \to +\infty$, while M_z stays uniformly bounded with respect to z. The integral kernels of L_z and M_z will be denoted by $\mathcal{L}_z$ and $\mathcal{M}_z$, respectively.

Notice that it is enough to consider $z \in \mathcal{S}$ since, according to Theorem 21.2, every eigenvalue of H_ε belongs to the half-strip $\mathcal{S}$ provided that ε is small enough.

In this paper, motivated by the asymptotic expansions (21.24), we use the decomposition (21.56) with the singular part L_z given by the integral kernel

$$\mathcal{L}_z(x,y) := \sqrt{\Re z}\,|V|^{1/2}(x)\,e^{-i\sqrt{\Re z}\,(x+y)}\,V_{1/2}(y)\,. \tag{21.57}$$

Properties of M_z are then stated in the following lemma.

Lemma 21.4. *For all $z \in \mathcal{S}$ and $(x,y) \in \mathbb{R}^2$, the integral kernel of the operator M_z defined by* (21.56) *with* (21.57) *satisfies*

$$\mathcal{M}_z(x,y) = \frac{1}{2}|V|^{1/2}(x)e^{-i\sqrt{\Re z}\,(x+y)}\big[\Im z\,(x+y) - (|x|+|y|)\big]V_{1/2}(y) + m_z(x,y)\,, \tag{21.58}$$

where for some $k > 0$, the function m_z satisfies, for all $z \in \mathcal{S}$ such that $\Re z \ge 1$,

$$|m_z(x,y)| \le \frac{k}{\sqrt{\Re z}}\,|V|^{1/2}(x)\,(1+x^2+y^2)\,|V|^{1/2}(y)\,. \tag{21.59}$$

If $V \in L^1\big(\mathbb{R}, (1+x^4)\,dx\big)$, then $\|M_z\|_{\mathrm{HS}}$ is uniformly bounded with respect to $z \in \mathcal{S}$.

Proof. In the following computations we assume $\Re z \ge 1$.

First, let $x \ge 0$ and $y \le 0$. Then, according to (21.13) and the asymptotic behaviour of $k_+(z)$ and $k_-(z)$ given in (21.24),

$$\mathcal{R}_z(x,y) = \frac{1}{k_+(z)+k_-(z)}\,e^{-k_+(z)\,x + k_-(z)\,y} = e^{-k_+(z)\,x+k_-(z)\,y}\big(\sqrt{\Re z} + \delta_1(z)\big)\,,$$

where $\delta_1(z)$ does not depend on (x,y) and $\delta_1(z) = \mathcal{O}(1/\sqrt{\Re z})$. Thus,

$$\begin{aligned}\mathcal{M}_z(x,y) = {} & \sqrt{\Re z}\,|V|^{1/2}(x)\,e^{-i\sqrt{\Re z}\,(x+y)}\left(e^{\Lambda_z(x,y)} - 1\right)V_{1/2}(y) \\ & + \delta_1(z)\,|V|^{1/2}(x)\,e^{-k_+(z)\,x+k_-(z)\,y}\,V_{1/2}(y)\,,\end{aligned} \tag{21.60}$$

where

$$\Lambda_z(x,y) := \left(-k_+(z) + i\sqrt{\Re z}\right)x + \left(k_-(z) + i\sqrt{\Re z}\right)y\,.$$

Writing a Taylor expansion for the two real-valued functions

$$[0,1] \ni t \longmapsto \Re e^{t\Lambda_z(x,y)} \qquad \text{and} \qquad [0,1] \ni t \longmapsto \Im e^{t\Lambda_z(x,y)}\,,$$

we obtain that, for some $t_1, t_2 \in [0,1]$,

$$e^{\Lambda_z(x,y)} - 1 = \Lambda_z(x,y) + \frac{1}{2}\Big[\Re\big(\Lambda_z(x,y)^2 e^{t_1\Lambda_z(x,y)}\big) + i\,\Im\big(\Lambda_z(x,y)^2 e^{t_2\Lambda_z(x,y)}\big)\Big]\,. \tag{21.61}$$

Notice that, for all $z \in \mathcal{S}$, $x \geq 0$ and $y \leq 0$, $\Re\Lambda_z(x,y) \leq 0$, hence

$$\frac{1}{2}\Big|\Re\big(\Lambda_z(x,y)^2 e^{t_1\Lambda_z(x,y)}\big) + i\,\Im\big(\Lambda_z(x,y)^2 e^{t_2\Lambda_z(x,y)}\big)\Big| \leq |\Lambda_z(x,y)|^2\,. \tag{21.62}$$

Moreover, due to (21.24), we have

$$\Lambda_z(x,y) = \frac{(\Im z - 1)\,x + (\Im z + 1)\,y}{2\sqrt{\Re z}} + \frac{\beta_z\,x + \gamma_z\,y}{(\Re z)^{3/2}}\,,$$

for some complex constants β_z and γ_z independent of (x,y) and uniformly bounded with respect to z. As a consequence, (21.61) and (21.62) yield

$$e^{\Lambda_z(x,y)} - 1 = \frac{1}{\sqrt{\Re z}}\left(\frac{(\Im z - 1)\,x + (\Im z + 1)\,y}{2} + \delta_2(z;x,y)\right),$$

where, for all $z \in \mathcal{S}$, $x \geq 0$ and $y \leq 0$,

$$|\delta_2(z;x,y)| \leq C_0\,\frac{1 + x^2 + y^2}{\sqrt{\Re z}}\,,$$

with some $C_0 > 0$. Summing up, (21.60) reads

$$\mathcal{M}_z(x,y) = |V|^{1/2}(x)\left(\tilde{\mathcal{M}}_z^0(x,y) + r_z(x,y)\right)V_{1/2}(y)\,, \tag{21.63}$$

where ($x \geq 0$, $y \leq 0$)

$$\begin{aligned}\tilde{\mathcal{M}}_z^0(x,y) &:= \frac{1}{2}\,e^{-i\sqrt{\Re z}\,(x+y)}\,\big[(\Im z - 1)\,x + (\Im z + 1)\,y\big]\\ &= \frac{1}{2}\,e^{-i\sqrt{\Re z}\,(x+y)}\,\big[\Im z\,(x+y) - (|x| + |y|)\big]\end{aligned} \tag{21.64}$$

and

$$r_z(x,y) := e^{-i\sqrt{\Re z}\,(x+y)}\,\delta_2(z;x,y) + e^{-k_+(z)\,x + k_-(z)\,y}\,\delta_1(z) \tag{21.65}$$

satisfies, with some positive constant C,

$$\forall z \in \mathcal{S}\,,\ x \geq 0\,,\ y \leq 0\,, \quad |r_z(x,y)| \leq \frac{C}{\sqrt{\Re z}}\,(1 + x^2 + y^2)\,. \tag{21.66}$$

By a similar analysis, we get the decomposition of the form (21.63) for $x \leq 0$ and $y \geq 0$ as well, where ($x \leq 0$, $y \geq 0$)

$$\begin{aligned}\tilde{\mathcal{M}}_z^0(x,y) &:= \frac{1}{2}e^{-i\sqrt{\Re z}\,(x+y)}\big[(\Im z + 1)\,x + (\Im z - 1)\,y\big]\\ &= \frac{1}{2}e^{-i\sqrt{\Re z}\,(x+y)}\big[\Im z\,(x+y) - (|x| + |y|)\big]\end{aligned} \tag{21.67}$$

and the bound (21.66) holds also for $x \leq 0$, $y \geq 0$.

The case $xy \geq 0$ can also be treated alike, by noticing that in this case the first term on the right-hand side of (21.13) satisfies

$$\left|\frac{1}{2k_\pm(z)}\,e^{-k_\pm(z)|x-y|}\right| \leq \frac{C'}{\sqrt{\Re z}}$$

with some $C' > 0$. Moreover, using (21.24),

$$\begin{aligned}&\pm\,\frac{k_+(z) - k_-(z)}{2k_\pm(z)\big(k_+(z) + k_-(z)\big)}\,e^{-k_\pm(z)(|x|+|y|)} - \sqrt{\Re z}\,e^{-i\sqrt{\Re z}\,(x+y)}\\ &\qquad\qquad = \frac{1}{2}\,e^{-i\sqrt{\Re z}\,(x+y)}\,\big[\Im z\,(x+y) - (|x| + |y|)\big] + \rho_z(x,y)\,,\end{aligned}$$

where $\rho_z(x,y)$ satisfies the bound (21.66). The decomposition (21.58) with (21.59) is therefore proved.

To complete the proof of the lemma, it remains to prove the uniform boundedness of $\mathcal{M}_z$. This can be deduced from (21.58) and (21.59). Indeed, with some $C_1 > 0$, we have, for $\Re z \geq 1$,

$$\|M_z\|_{\mathrm{HS}}^2 \leq C_1 \int_{\mathbb{R}^2} |V(x)|\,(1+x^2+y^2)^2\,|V(y)|\,dx\,dy\,,$$

where the right hand side is finite if $V \in L^1(\mathbb{R},(1+x^4)\,dx)$ and actually independent of z. If $\Re z \leq 1$, then according to (21.55) and the expression (21.57) of the kernel $\mathcal{L}_z$, we have

$$\|M_z\|_{\mathrm{HS}} \leq \|K_z\|_{\mathrm{HS}} + \|L_z\|_{\mathrm{HS}} \leq C_2 \sqrt{\int_{\mathbb{R}^2} |V(x)|\,(1+|x|+|y|)^2\,|V(y)|\,dx\,dy}$$

with some $C_2 > 0$, hence the norm $\|M_z\|_{\mathrm{HS}}$ is uniformly bounded for $\Re z \leq 1$ as well. □

Remark 21.5. Using a first-order expansion in (21.61) instead of the second-order expansion, we would obtain the uniform boundedness of M_z under the weaker assumption $V \in L^1\big(\mathbb{R},(1+x^2)\,dx\big)$. However, the second-order expansion in (21.61) is required in order to get the exact expression (21.64) of the principal term $\tilde{\mathcal{M}}_z^0(x,y)$ in (21.63).

Since $\|M_z\|$ is uniformly bounded with respect to $z \in \mathcal{S}$, the operator $(1+\varepsilon M_z)$ is boundedly invertible for all ε small enough. Consequently, in view of the identity

$$\varepsilon K_z + 1 = \varepsilon(L_z + M_z) + 1 = (1+\varepsilon M_z)\big[\varepsilon(1+\varepsilon M_z)^{-1}L_z + 1\big]$$

and Theorem 21.4, we have (for all $z \in \mathcal{S}$)

$$z \in \sigma_{\mathrm{p}}(H_\varepsilon) \quad \Longleftrightarrow \quad -1 \in \sigma\big(\varepsilon(1+\varepsilon M_z)^{-1}L_z\big)\,. \tag{21.68}$$

From the definition (21.57) we see that L_z is a rank-one operator. Consequently, $\varepsilon(1+\varepsilon M_z)^{-1}L_z$ is of rank one too. Indeed, for all $f \in L^2(\mathbb{R})$, we have

$$\varepsilon(1+\varepsilon M_z)^{-1}L_z f = \varepsilon\sqrt{\Re z}\,(f,\bar{\psi}_z)\,(1+\varepsilon M_z)^{-1}\phi_z\,,$$

where

$$\phi_z(x) := e^{-i\sqrt{\Re z}\,x}\,|V|^{1/2}(x) \qquad \text{and} \qquad \psi_z(x) := e^{-i\sqrt{\Re z}\,x}\,V_{1/2}(x)\,.$$

It follows that $\varepsilon(1+\varepsilon M_z)^{-1}L_z$ has the unique non-zero eigenvalue

$$\varepsilon\sqrt{\Re z}\,\big((1+\varepsilon M_z)^{-1}\phi_z,\bar{\psi}_z\big)\,.$$

Equivalence (21.68) thus reads

$$z \in \sigma_{\mathrm{p}}(H_\varepsilon) \quad \Longleftrightarrow \quad -1 = \varepsilon\sqrt{\Re z}\,\big((1+\varepsilon M_z)^{-1}\phi_z,\bar{\psi}_z\big)\,. \tag{21.69}$$

Note that the right hand side represents an implicit equation for z.

Writing

$$(1+\varepsilon M_z)^{-1} = \sum_{j=0}^{n-1}(-1)^j\varepsilon^j M_z^j + (-1)^n\varepsilon^n M_z^n(1+\varepsilon M_z)^{-1}\,,$$

the condition on the right hand side of (21.69) reads

$$\frac{1}{\sqrt{\Re z}} = \sum_{j=1}^{n}(-1)^j\,\big(M_z^{j-1}\phi_z,\bar{\psi}_z\big)\,\varepsilon^j + (-1)^{n+1}\,\big(M_z^n(1+\varepsilon M_z)^{-1}\phi_z,\bar{\psi}_z\big)\,\varepsilon^{n+1}\,. \tag{21.70}$$

In the following we estimate each term on the right hand side of (21.70).

For $j = 1,\dots,n$, denoting

$$V^{\otimes j}(x_1,\dots,x_j) := V(x_1)\dots V(x_j)\,,$$

and using the decomposition (21.60) with (21.67), we have

$$\begin{aligned}
\big(M_z^{j-1}\phi_z, \bar\psi_z\big) &= \int_{\mathbb{R}^j} \mathcal{M}_z(x_1,x_2)\ldots\mathcal{M}_z(x_{j-1},x_j)\,\phi_z(x_j)\,\psi_z(x_1)\,dx_1\ldots dx_j \\
&= \int_{\mathbb{R}^j}\left(\prod_{\ell=1}^{j-1}|V|^{1/2}(x_\ell)\big[\tilde{\mathcal{M}}_z^0(x_\ell,x_{\ell+1})+r_z(x_\ell,x_{\ell+1})\big]V_{1/2}(x_{\ell+1})\right) \\
&\quad\times |V|^{1/2}(x_j)\,e^{-i\sqrt{\Re z}\,(x_1+x_j)}\,V_{1/2}(x_1)\,dx_1\ldots dx_j \\
&= \int_{\mathbb{R}^j} e^{-i\sqrt{\Re z}\,(x_1+x_j)}\,V^{\otimes j}(x_1,\ldots,x_j) \\
&\quad\times\prod_{\ell=1}^{j-1}\big[\tilde{\mathcal{M}}_z^0(x_\ell,x_{\ell+1})+r_z(x_\ell,x_{\ell+1})\big]\,dx_1\ldots dx_j \\
&= I_{j-1}(z)+R_{j-1}(z)\,,
\end{aligned} \tag{21.71}$$

where

$$\begin{aligned}
I_{j-1}(z) := \frac{1}{2^{j-1}}\int_{\mathbb{R}^j} & e^{-2i\sqrt{\Re z}\,\sum_{\ell=1}^{j} x_\ell}\,V^{\otimes j}(x_1,\ldots,x_j) \\
&\times\prod_{\ell=1}^{j-1}\big[\Im z\,(x_\ell+x_{\ell+1})-(|x_\ell|+|x_{\ell+1}|)\big]\,dx_1\ldots dx_j
\end{aligned} \tag{21.72}$$

and $R_{j-1}(z) := (M_z^{j-1}\phi_z,\bar\psi_z) - I_{j-1}(z)$ contains all the integral terms involving at least one factor of the form $r_z(x_\ell,x_{\ell+1})$. Using (21.66), one can easily check that

$$R_{j-1}(z) = \mathcal{O}\left(\frac{1}{\sqrt{\Re z}}\right) \tag{21.73}$$

whenever $V\in L^1(\mathbb{R},(1+x^{2n})\,dx)$.

On the other hand, we have

$$\prod_{\ell=1}^{j-1}\big[\Im z\,(x_\ell+x_{\ell+1})-(|x_\ell|+|x_{\ell+1}|)\big] = \sum_{\vec\ell\in\mathcal{J}_{j-1}}\prod_{m=1}^{j-1}(\Im z\,x_{\ell_m}-|x_{\ell_m}|)\,,$$

for a subset $\mathcal{J}_{j-1}\subset\{1,\ldots,j\}^{j-1}$ such that, for all $\vec\ell\in\mathcal{J}_{j-1}$, each coordinate in $\vec\ell$ is repeated at most twice. Consequently, separating the variables in (21.72), we get, for some positive integer M_j,

$$I_{j-1}(z) = \frac{1}{2^{j-1}}\sum_{k=1}^{M_j} I_{j-1}^{(k)}(z)\,, \tag{21.74}$$

where each term $I_{j-1}^{(k)}(z)$ has the form

$$\begin{aligned}
I_{j-1}^{(k)}(z) &= \left(\int_{\mathbb{R}} e^{-2i\sqrt{\Re z}\,x}\,V(x)\,dx\right)^{a_{k,j}} \\
&\quad\times\left(\int_{\mathbb{R}} e^{-2i\sqrt{\Re z}\,x}(\Im z\,x-|x|)\,V(x)\,dx\right)^{b_{k,j}} \\
&\quad\times\left(\int_{\mathbb{R}} e^{-2i\sqrt{\Re z}\,x}\,(\Im z\,x-|x|)^2 V(x)\,dx\right)^{c_{k,j}}\,,
\end{aligned}$$

with $a_{k,j}, b_{k,j}, c_{k,j}$ such that

$$\begin{cases} a_{k,j}>0\,,\ b_{k,j}\geq 0\,,\ c_{k,j}\geq 0\,, \\ a_{k,j}+b_{k,j}+c_{k,j}=j\,, \\ b_{k,j}+2c_{k,j}=j-1\,. \end{cases}$$

Thus, if $\mathcal{F}[f](\xi)$ denotes the Fourier transform of f at point ξ, we have

$$\begin{aligned}
I_{j-1}^{(k)}(z) &= \Big(\mathcal{F}[V](2\sqrt{\Re z})\Big)^{a_{k,j}}\Big(\mathcal{F}\big[(\Im z\,x-|x|)V(x)\big](2\sqrt{\Re z})\Big)^{b_{k,j}} \\
&\quad\times\Big(\mathcal{F}\big[(\Im z\,x-|x|)^2V(x)\big](2\sqrt{\Re z})\Big)^{c_{k,j}}\,.
\end{aligned} \tag{21.75}$$

Now, since for $s = 1,2$ the function $x \mapsto (\Im z\, x - |x|)^s V(x)$ belongs to $L^1(\mathbb{R})$ by assumption, its Fourier transform is in $L^\infty(\mathbb{R})$ and it is continuous. Hence there exists $M_1 > 0$ such that, for all $z \in \mathcal{S}$ and $s = 1,2$,

$$\left| \mathcal{F}\big[(\Im z\, x - |x|)^s V(x)\big](2\sqrt{\Re z}) \right| \leq M_1 \, .$$

Similarly, since $V \in W^{1,1}(\mathbb{R})$, the function $\xi \mapsto \xi\, \mathcal{F}[V](\xi)$ belongs to $L^\infty(\mathbb{R})$ and it is continuous. Hence there exists $M_2 > 0$ such that, for all $z \in \mathcal{S}$,

$$\left| \mathcal{F}[V](2\sqrt{\Re z}) \right| \leq \frac{M_2}{\sqrt{\Re z}} \, .$$

Thus (21.74) and (21.75) give

$$I_{j-1}(z) = \mathcal{O}\left(\frac{1}{\sqrt{\Re z}}\right) . \tag{21.76}$$

Finally, (21.71), (21.73) and (21.76) yield

$$\big(M_z^{j-1}\phi_z, \bar{\psi}_z\big) = \mathcal{O}\left(\frac{1}{\sqrt{\Re z}}\right)$$

for all $j = 1, \dots, n$. Thus, according to (21.70),

$$\frac{1}{\sqrt{\Re z}}\big(1 - \mathcal{O}(\varepsilon)\big) = (-1)^{n+1}\big(M_z^n(1+\varepsilon M_z)^{-1}\phi_z, \bar{\psi}_z\big)\,\varepsilon^{n+1} \, ,$$

uniformly with respect to z as $\varepsilon \to 0$. We then notice that the right hand side in the above identity has the form $\mathcal{O}(\varepsilon^{n+1})$, uniformly with respect to z, as $\varepsilon \to 0$. Therefore, we have

$$\frac{1}{\sqrt{\Re z}} = \mathcal{O}(\varepsilon^{n+1}) \, ,$$

which concludes the proof of Theorem 21.3. □

21.7 Examples

21.7.1 Dirac interaction

In order to test our results on an explicitly solvable model, let us consider the operator formally given by the expression

$$H_\alpha = -\frac{d^2}{dx^2} + i\,\mathrm{sgn}(x) + \alpha\,\delta(x) \, , \qquad \alpha \in \mathbb{C} \, ,$$

where δ is the Dirac delta function. In fact, H_α can be rigorously defined (*cf* [20, Ex. 5.27]) as the m-sectorial operator in $L^2(\mathbb{R})$ associated with the form sum $h + \alpha v$, where

$$v(\psi,\phi) := \psi(0)\bar{\phi}(0) \, , \qquad \mathsf{D}(v) := W^{1,2}(\mathbb{R}) \, .$$

We have

$$\begin{aligned} (H_\alpha\psi)(x) &= -\psi''(x) + i\,\mathrm{sgn}(x)\,\psi(x) \quad \text{for a.e. } x \in \mathbb{R} \, , \\ \mathsf{D}(H_\alpha) &= \left\{\psi \in W^{1,2}(\mathbb{R}) \cap W^{2,2}(\mathbb{R}\setminus\{0\}) : \ \psi'(0^+) - \psi'(0^-) = \alpha\,\psi(0)\right\} \, . \end{aligned}$$

It is also possible to show that H_α is $\mathcal{T}$-self-adjoint.

Using for instance [12, Corol. IX.4.2], we have the stability result

$$\sigma_{\mathrm{ess}}(H_\alpha) = \sigma_{\mathrm{ess}}(H) = [0,+\infty) + i\,\{-1,+1\}$$

for all $\alpha \in \mathbb{C}$. Since H_α is $\mathcal{T}$-self-adjoint, the residual spectrum of H_α is empty (*cf* [20, Sec. 5.2.5.4]). Finally, the eigenvalue problem for H_α can be solved explicitly and we find that H_α possesses a unique (discrete) eigenvalue given by

$$\lambda(\alpha) := \frac{1}{\alpha^2} - \frac{\alpha^2}{4} \tag{21.77}$$

if, and only if,

$$\lambda(\alpha) \notin [0,+\infty) + i\,\{-1,+1\} \, . \tag{21.78}$$

In particular, the eigenvalue exists for all $\alpha \in \mathbb{R} \setminus \{0\}$ and in this case it is real. It is interesting that the rate at which $\lambda(\alpha)$ tends to infinity as $\alpha \to 0$ coincides with the bound of Theorem 21.2, even if this theorem does not apply to the present singular potential and even for non-real α.

Now, in order to state the condition (21.78) more explicitly in terms of α, let us set, for all $\sigma = (\sigma_1, \sigma_2, \sigma_3) \in \{-1, +1\}^3$,

$$\Gamma_\sigma := \left\{ \sigma_1 \sqrt{-2(r + i\sigma_2) + 2\sigma_3 \sqrt{r(r + 2i\sigma_2)}} \; : \; r \in [0, +\infty) \right\} .$$

Notice that, for all $r \in [0, +\infty)$, the square roots in the expression above are well defined. Then the condition (21.78) is equivalent to $\alpha \notin \Gamma$, where

$$\Gamma := \bigcup_{\sigma \in \{-1,+1\}^3} \Gamma_\sigma \, . \tag{21.79}$$

The curve Γ is represented in Figure 21.3.

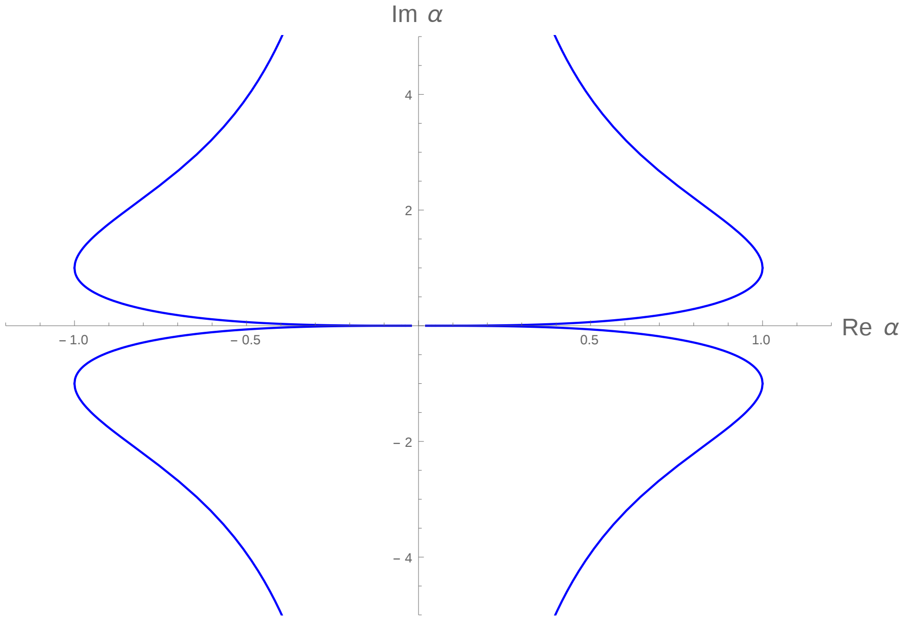

Figure 21.3: The curve Γ in the complex plane representing values of α for which the eigenvalue of H_α does not exist.

Let us summarise the spectral properties into the following proposition.

Proposition 21.4. *For any* $\alpha \in \mathbb{C}$, *we have*

$$\sigma_{\mathrm{r}}(H_\alpha) = \varnothing \, ,$$
$$\sigma_{\mathrm{c}}(H_\alpha) = [0, +\infty) + i \, \{-1, +1\} \, ,$$
$$\sigma_{\mathrm{p}}(H_\alpha) = \begin{cases} \varnothing & \textit{if} \quad \alpha \in \Gamma \, , \\ \{\lambda(\alpha)\} & \textit{if} \quad \alpha \notin \Gamma \, , \end{cases}$$

where $\lambda(\alpha)$ *is given by* (21.77) *and* Γ *is the domain defined in* (21.79).

21.7.2 Step-like potential

To have a definitive support for the existence of discrete spectra for the operators of the type (21.8), here we consider $\varepsilon = 1$ and the following step-like profile for the perturbing potential:

$$V_{a,b}(x) := (-i \; \mathrm{sgn}(x) - b) \, \chi_{[-a,a]}(x) \, ,$$

where $a > 0$ and $b \in \mathbb{C}$. We set $H_{a,b} := H + V_{a,b}$. By Proposition 21.3,

$$\sigma_{\mathrm{ess}}(H_{a,b}) = [0, +\infty) + i \, \{-1, +1\} \tag{21.80}$$

for all $a > 0$ and $b \in \mathbb{C}$.

The differential equation of the eigenvalue problem $H_{a,b}\psi = \lambda\psi$ can be solved in terms of sines and cosines in each of the intervals $(-\infty, -a)$, $(-a, a)$ and $(a, +\infty)$. Choosing integrable solutions in the infinite intervals and gluing the respective solutions at $\pm a$ by requiring the $W^{2,2}$-regularity, we arrive at the following equation

$$\left[\sqrt{\lambda^2+1} - \lambda - b\right] \frac{\sin\left(2a\sqrt{\lambda+b}\right)}{\sqrt{\lambda+b}} - i\left(\sqrt{\lambda+i} - \sqrt{\lambda-i}\right) \cos\left(2a\sqrt{\lambda+b}\right) = 0 \tag{21.81}$$

for eigenvalues λ satisfying $|\Im\lambda| < 1$ and $\lambda + b \notin (-\infty, 0)$. The equation for the case $\lambda = -b$ is recovered after taking the limit $\lambda \to -b$ in the above equation. For eigenvalues λ satisfying $|\Im\lambda| < 1$ and $\lambda + b \in (-\infty, 0)$, we find

$$\left[\sqrt{\lambda^2+1} - \lambda - b\right] \frac{\sinh\left(2a\sqrt{|\lambda+b|}\right)}{\sqrt{|\lambda+b|}} - i\left(\sqrt{\lambda+i} - \sqrt{\lambda-i}\right) \cosh\left(2a\sqrt{|\lambda+b|}\right) = 0\,.$$

In the same manner, it is possible to derive equations for eigenvalues λ satisfying $|\Im\lambda| \geq 1$. However, we shall not present these formulae, for below we are particularly interested in real eigenvalues. We only mention that it is easy to verify that no point in the essential spectrum (21.80) can be an eigenvalue.

Henceforth, we investigate the existence of real eigenvalues. Moreover, we restrict to real b and look for eigenvalues $\lambda > -b$, so that it is enough to work with (21.81). First of all, notice that, for any $\lambda > -b$ satisfying (21.81), $\sin\left(2a\sqrt{\lambda+b}\right)$ never vanishes. At the same time, $\Im\sqrt{\lambda+i}$ is non-zero for real λ. We can thus rewrite (21.81) as follows

$$\cot\left(2a\sqrt{\lambda+b}\right) = -\frac{\sqrt{\lambda^2+1} - (\lambda+b)}{2\sqrt{\lambda+b}\,\Im\sqrt{\lambda+i}} \sim b \qquad \text{as} \quad \lambda \to +\infty\,.$$

Since there is a periodic function with range $\mathbb{R}$ on the left hand side, it follows from the asymptotics that $H_{a,b}$ possesses infinitely many eigenvalues for every real b. Let us highlight this result by the following proposition.

Proposition 21.5. *For any $a > 0$ and $b \in \mathbb{R}$, $H_{a,b}$ possesses infinitely many distinct real discrete eigenvalues.*

Several real eigenvalues of $H_{a,b}$ as functions of $b \in \mathbb{R}$ are represented in Figure 21.4.

21.7.3 Dirichlet realisation

Since the spectrum of H is the union of the two half-lines $\mathbb{R}_+ + i$ and $\mathbb{R}_+ - i$, one might have expected the operator H to behave as some sort of decoupling of two operators $-\frac{d^2}{dx^2} + i$ in $L^2(\mathbb{R}_+)$ and $-\frac{d^2}{dx^2} - i$ in $L^2(\mathbb{R}_-)$. The existence of non-trivial pseudospectra (*cf* Theorem 21.1) actually indicates that this is not the case. Indeed, the situation strongly depends on the way the operator is defined, emphasising the importance of the choice of domain in the pseudospectral behaviour of an operator.

For comparison, let H^D be the operator in $L^2(\mathbb{R})$ that acts as H in $\mathbb{R}_+^* := (0, +\infty)$ and $\mathbb{R}_-^* := (-\infty, 0)$, but satisfies an extra Dirichlet condition at zero, *i.e.*,

$$\mathsf{D}(H^D) := \left(W^{2,2} \cap W_0^{1,2}\right)\left(\mathbb{R} \setminus \{0\}\right).$$

Considering this operator instead of H means that the previous matching conditions at $x = 0$, $u(0^-) = u(0^+)$ and $u'(0^-) = u'(0^+)$ for $u \in \mathsf{D}(H)$, are replaced by the conditions $u(0^-) = 0 = u(0^+)$ for $u \in \mathsf{D}(H^D)$.

We can write H^D as a direct sum

$$H^D = H_-^D \oplus H_+^D\,, \tag{21.82}$$

where $H_\pm^D$ are operators in $L^2(\mathbb{R}_\pm^*)$ defined by

$$H_\pm^D := -\frac{d^2}{dx^2} \pm i\,, \qquad \mathsf{D}(H_\pm^D) := \left(W^{2,2} \cap W_0^{1,2}\right)(\mathbb{R}_\pm^*)\,. \tag{21.83}$$

Since the spectra of $H_\pm^D$ are trivially found, we therefore have (see [12, Sec. IX.5])

$$\sigma(H^D) = \sigma(H_-^D) \cup \sigma(H_+^D) = \mathbb{R}_+ + i\,\{-1, +1\}\,.$$

Hence H^D and H have the same spectrum (*cf* Proposition 21.1).

We can also decompose the resolvent of H_D as follows

$$(H^D - z)^{-1} = (H_-^D - z)^{-1} \oplus (H_+^D - z)^{-1}$$

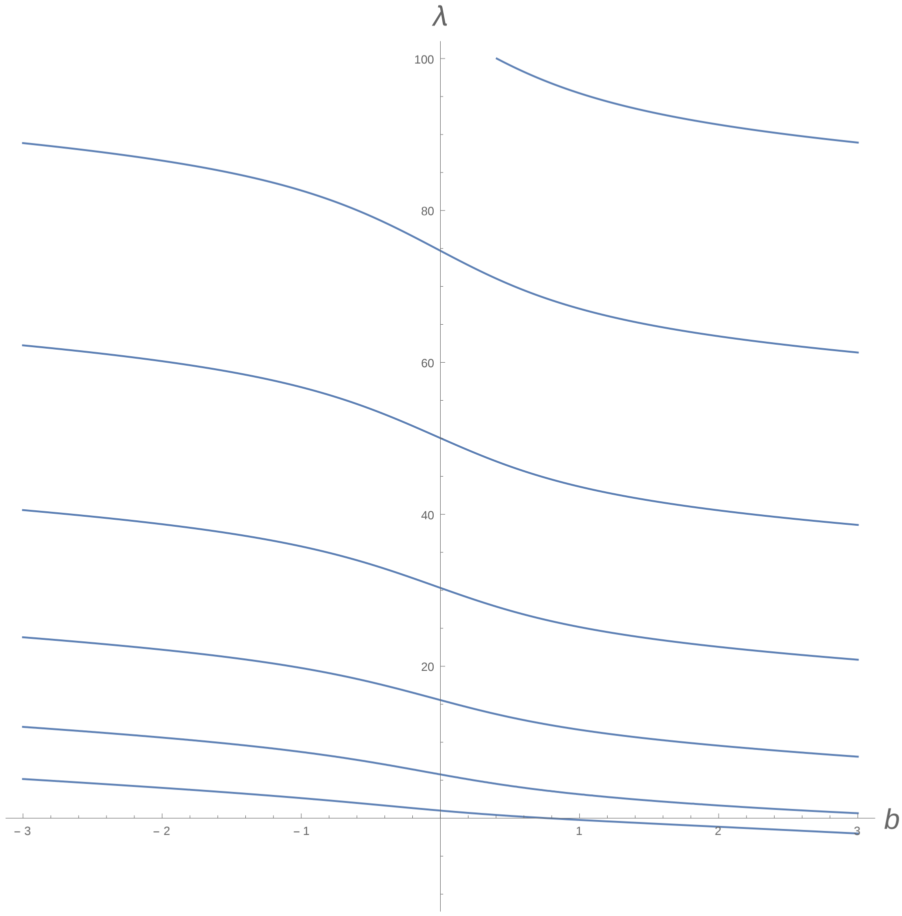

Figure 21.4: Dependence of real eigenvalues of $H_{a,b}$ on b for $a = 1$.

for every $z \notin \mathbb{R}_+ + i\{-1, +1\}$. Since $H^D_\pm$ are obtained from self-adjoint operators shifted by a constant, they both have trivial pseudospectra. Consequently, H^D has trivial pseudospectra as well. In other words, although H^D and H have the same spectrum, that of H is far more unstable (*cf* Theorem 21.1).

To be more specific, let us write down the integral kernel $\mathcal{R}^D_z$ of $(H^D - z)^{-1}$. For $f \in L^2(\mathbb{R})$, the function $(H^D - z)^{-1} f$ has the form (21.15), where the constants A_+, A_-, B_+, B_- are uniquely determined by the Dirichlet condition at 0 together with the condition $(H^D - z)^{-1} f(x) \to 0$ as $x \to \pm\infty$. The former yields $B_+ = -A_+$ and $B_- = -A_-$, while the latter gives the following values for A_+ and A_-:

$$A_+ = \frac{1}{2k_+(z)} \int_0^{+\infty} f(y)\, e^{-k_+(z)y}\, dy\,, \qquad A_- = -\frac{1}{2k_-(z)} \int_{-\infty}^{0} f(y)\, e^{k_+(z)y}\, dy\,.$$

Eventually, we obtain the following expression for the integral kernel:

$$\mathcal{R}^D_z(x, y) = \frac{1}{2k_\pm(z)} \left(e^{-k_\pm(z)|x-y|} - e^{-k_\pm(z)(|x|+|y|)} \right) \chi_{\mathbb{R}_\pm}(y)\,, \qquad \pm x > 0\,.$$

Now, as in Section 21.5.1, we can consider the perturbed operator

$$H^D_\varepsilon := H^D \dot{+} \varepsilon V$$

for any $V \in L^1(\mathbb{R})$. We claim that, under the additional assumption $V \in L^1(\mathbb{R}, (1+x^2)\, dx)$, the Hilbert-Schmidt norm of the Birman-Schwinger operator

$$K^D_z := |V|^{1/2} (H^D - z)^{-1} V_{1/2}$$

is uniformly bounded with respect to $z \notin \mathbb{R}^+ + i\{-1, 1\}$. To see it, let us first assume $x > 0$. If $|z - i| \le c_0$ for some positive c_0, then

$$\begin{aligned} |\mathcal{R}^D_z(x, y)| &\le \frac{1}{2|k_+(z)|} \left(\left| e^{-k_+(z)|x-y|} - 1 \right| + \left| (e^{-k_+(z)(|x|+|y|)} - 1 \right| \right) \\ &\le \frac{|x - y| + |x| + |y|}{2}\,, \end{aligned}$$

where we have used the inequality $|e^{-\omega} - 1| \leq |\omega|$ for $\Re\omega \geq 0$. On the other hand, if $|z - i| > c_0$, then $|k_+(z)|$ is uniformly bounded from below, hence $\mathcal{R}_z^D(x,y)$ is uniformly bounded with respect to $x \geq 0$, $y \in \mathbb{R}$ and z such that $|z - i| > c_0$. The same analysis can be performed for $x < 0$, thus there exists $C > 0$ such that, for all $(x,y) \in \mathbb{R}^2$ and $z \notin [0,+\infty) + i\{-1,1\}$,

$$|\mathcal{R}_z^D(x,y)| \leq C(1 + |x| + |y|)\,.$$

Consequently, the computation of the Hilbert-Schmidt norm of K_z^D yields

$$\|K_z^D\|_{\mathrm{HS}} \leq C \int_{\mathbb{R}} (1 + x^2)|V(x)|\,dx\,. \tag{21.84}$$

After noticing that $\sigma_{\mathrm{ess}}(H_\varepsilon^D) = \sigma_{\mathrm{ess}}(H^D)$ for all $\varepsilon \in \mathbb{R}$ (by the same arguments as in the proof of Proposition 21.3), the Birman-Schwinger principle (*i.e.* a version of Theorem 21.4 for H_ε^D) leads to the following statement.

Proposition 21.6. *Let $V \in L^1\big(\mathbb{R}, (1 + x^2)\,dx\big)$. There exists a positive constant $\varepsilon_0 > 0$ such that, for all $\varepsilon \in (0, \varepsilon_0)$, we have*

$$\sigma(H_\varepsilon^D) = \sigma(H^D) = \mathbb{R}_+ + i\,\{-1,1\}\,.$$

In other words, in the simpler situation of the operator H^D, we are able to prove the absence of weakly coupled eigenvalues. Proposition 21.6 can be considered as some sort of “Hardy inequality” or “absence of virtual bound state” for the non-self-adjoint operator H^D. Let us also notice that a similar result has been established by Frank [13] in the case of Schrödinger operators with complex potentials in three and higher dimensions.

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Chapter 22

Pseudomodes for Schrödinger operators with complex potentials

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Joint work with: Petr Siegl

Pseudomodes for Schrödinger operators with complex potentials

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Abstract. For one-dimensional Schrödinger operators with complex-valued potentials, we construct pseudomodes corresponding to large pseudoeigenvalues. We develop a first systematic non-semi-classical approach, which results in a substantial progress in achieving optimal conditions and conclusions as well as in covering a wide class of previously inaccessible potentials, including discontinuous ones. Applications of the present results to higher-dimensional Schrödinger operators are also discussed.

Keywords: pseudospectrum, Schrödinger operators, complex potential, WKB
MSC (2010): 34E20, 34L40, 35P20, 47A10, 81Q12, 81Q20

22.1 Introduction

While the spectral theorem reduces the study of self-adjoint operators to a spectral analysis, it is well known that the spectrum of a non-normal operator provides by far insufficient information about its properties. It is not the spectrum that determines the decay of the associated heat semigroup and the behaviour of eigenvalues under small perturbations, but rather the *pseudospectrum*, which measures the largeness of the resolvent, see *e.g.* [20, 6, 11].

The ε-pseudospectrum of a closed operator H consists of the union of its spectrum and complex points λ satisfying $\|(H-\lambda)f\| < \varepsilon \|f\|$ for some vector f from the domain of H. The number λ and the vector f are respectively called the *pseudoeigenvalue* (or *approximate eigenvalue*) and *pseudoeigenvector* (or *pseudomode*) of H. The pseudoeigenvalues of H may be turned into genuine eigenvalues of the perturbed operator $H + L$ with $\|L\| < \varepsilon$ and they can lie outside (in fact "very far" from) the ε-tubular neighbourhood of the spectrum of H if the operator is not normal. This is the well-known *spectral instability* of non-normal operators under small perturbations.

This paper is concerned with a study, in several aspects complete, of approximate eigenvalues and pseudomodes of the one-dimensional Schrödinger operators

$$H_V := -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + V(x)\,, \tag{22.1}$$

where V is a *complex*-valued function. We consider L^2-realisations of H_V on the whole line $\mathbb{R}$ or the semi-axis $\mathbb{R}_+$, the latter having immediate consequences for the multi-dimensional operators with radial potentials and their perturbations. Thus our objective is to construct a λ-dependent family of pseudomodes f_λ such that

$$\|(H_V-\lambda)f_\lambda\| = o(1)\,\|f_\lambda\| \qquad \text{as} \qquad \lambda\to\infty \quad \text{in} \quad \Omega\subset\mathbb{C}. \tag{22.2}$$

The abstract self-adjoint theory yields immediately that real-valued potentials V are irrelevant here, since then (22.2) may hold only when λ approaches the spectrum of H_V. On the other hand, the by now well-known examples of potentials for which (22.2) holds in vast complex regions Ω are just purely imaginary monomials $V(x) := ix^n$ and their perturbations, see *e.g.* [5, 4, 18, 19, 12, 16]. Hence, the state of the art of the current research in construction of the "large-energy" pseudomodes for (non-semiclassical) Schrödinger operators is by far incomplete and the objective of this paper is to fill up the gap. In fact, all known cases (as well as all semi-classical ones) represent the simplest illustrations of our results, see Examples 22.1, 22.9 and 22.10.

The fundamental questions that we address here read as follows:

- For which potentials there is a non-trivial region $\Omega\subset\mathbb{C}$ where (22.2) holds?
- Comparing to $\Im V$, how large can $\Re V$ be so that (22.2) is preserved?
- Depending on V, what is the shape of Ω?
- Is the polynomial-like character of the so far studied operators important?

- What is the role of the regularity of V?

Basically all available results on non-trivial pseudospectra of Schrödinger operators are deduced by scaling from *semiclassical pseudomodes*, where a small parameter h^2 is added in front of the second-derivative in (22.2), see *e.g.*, [5, 7]. However, such an approach has several drawbacks. First of all, only very specific (homogeneous or their perturbations) potentials can be treated and unboundedness of $\Im V$ at infinity may seem to be crucial due to the scaling. Second, the artificial transition to the new parameter h, related in various ways to λ, complicates the natural interpretation of the results as well as the main points in the proofs. Finally, with the exception of the *imaginary shifted harmonic oscillator* $V(x) := (x+i)^2$ treated in [12], no claims seem to be available when $\Re V$ is larger than $\Im V$ at infinity. For these reasons, in this paper we attack the problem directly (without introducing the semiclassical parameter h) and provide several answers to the aforementioned questions.

The present results have also a connection to some open problems posed during the 2015 AIM workshop [1]. In particular, we would like to emphasise the following insights provided by this paper.

The semiclassical setting as a consequence

From our approach the known claims in the semiclassical setting follow immediately. In particular, the Davies' condition [5] $\Im V' \neq 0$ or its (weaker) versions (see [21, 17]) can be easily generalised, see Example 22.10. It is also worth noting that our general non-semiclassical pseudomodes do not always localise, instead their support may extend.

Optimality of potentials

Our assumption (22.30) on the allowed size of $\Re V$ is optimal, at least for polynomial-like potentials (with $\nu_\pm = -1$ in assumption (22.29)). Indeed, by completely different methods, it has been established in [14, 15] that *e.g.* for potentials V satisfying $\Re V(x) = |x|^\beta$ with $\beta \geq 1$ and

$$\exists \epsilon > 0, \quad |\Im V(x)|^2 = \mathcal{O}(|x|^{\beta-2-\epsilon}), \quad |x| \to \infty, \tag{22.3}$$

the eigensystem of H_V contains a Riesz basis (and only a finitely many multiple eigenvalues) and hence the only non-trivial pseudomodes exist for λ close to the eigenvalues of H_V (with known asymptotics, see [14]). In turn, the current results suggest that the condition (22.3) is optimal with respect to the Riesz basis property of H_V (which can be indeed concluded if more information about the position of eigenvalues of H_V is available) and confirms that the borderline case (potentials with $\epsilon = 0$ in (22.3)) is the most challenging one, see [1, Open Problem 15.1]. Moreover, the assumption (22.30) has a very natural interpretation, namely, the pseudomodes loose their exponential decay if (22.30) is not satisfied, see Remark 22.2.

Optimality of pseudospectral regions

Our restrictions on the set Ω in (22.141), expressed in terms of conditions on $a := \Re\lambda$ and $b := \Im\lambda$, seem to be optimal. The optimality for the *rotated harmonic oscillator* $V(x) := ix^2$ follows by Boulton's conjecture [4] solved by Pravda-Starov [18], see Example 22.9. The lower bound of (22.156) is also known to be optimal for the *imaginary cubic oscillator* $V(x) := ix^3$, see [3, Sec. 4.1]. The study of optimality of our estimates on the region Ω in general cases constitute an interesting open problem.

Generality

We are able to treat a wide class of potentials being far beyond polynomial or scalable ones (we also allow a large $\Re V$ without restricting its sign). The method can be further straightforwardly generalised for even wilder potentials than already a quite wide range covered here (from bounded or even decaying, see Section 22.3.5, to super-exponential ones). For instance, the previously inaccessible (non-scalable) cases like $V(x) := i\sinh(x)$ or $V(x) := i\arctan(x)$ are included, see Examples 22.2 and 22.3. It is also important to stress that for realisations in $L^2(\mathbb{R})$, just the different asymptotic behaviour of $\Im V$ at $\pm\infty$:

$$\lim_{x\to-\infty} \Im V(x) \;\cdot\; \lim_{x\to+\infty} \Im V(x) \;<\; 0 \tag{22.4}$$

(see also (22.28) for a slight generalisation) is crucial to ensure the "significant non-self-adjointness" of H_V and thus the validity of (22.2) for $\lambda \to +\infty$. For decaying but non-integrable potentials V, condition (22.4) can be further weakened by requiring that $\Im V$ approaches 0 from opposite sides at $\pm\infty$, see Section 22.3.5. The various conditions of the type (22.4) can be viewed as a global version of the local Davies' condition $\Im V' \neq 0$ or its weaker versions mentioned above.

Rough potentials

In fact, we cover even *discontinuous* potentials, which were previously inaccessible to semiclassical techniques. This is achieved by developing a robust method of λ-dependent mollifications of the potential. This new idea enables us to eventually solve an open problem raised during the AIM workshop [1, Open Problem 10.1].

The regularity of potentials and decay rates of pseudomodes

We explicitly demonstrate the crucial influence of the regularity (or local deformations) of V on the best possible rates in (22.2). The latter was observed (although not proved due to the missing upper bounds on the resolvent) in the difference for analytic and smooth potentials (exponential versus "faster than any power" rates), see *e.g.* [5, 7]. In this paper we stress (and prove) the difference in rates for various step-like potentials of the type (arctan may be replaced by any "regularisation" of sgn)

$$V_1(x) := i\,\mathrm{sgn}(x) \qquad \text{versus} \qquad V_2(x) := i\arctan(x). \tag{22.5}$$

Here the best possible rate is linear in the first case (as proved in [9] by a careful analysis of the resolvent kernel) versus the "faster than any power" rate in the second case, see Example 22.3. Notice that the even more drastic local deformation, namely the operator $-\mathrm{d}^2/\mathrm{d}x^2 + i\,\mathrm{sgn}(x)$ subject to an *additional* Dirichlet boundary condition at 0, exhibits *no decay* for $\lambda \to +\infty$ in (22.2), since such an operator becomes normal.

Laptev-Safronov eigenvalue bounds

Our results for decaying potentials from Section 22.3.5 show that the bound on individual eigenvalues of one-dimensional Schrödinger operators due to Laptev and Safronov (see [13, Thm. 5] and [1, Open Problem 7.1]) cannot be improved using the Birman-Schwinger technique (since the norm estimate on the Birman-Schwinger operator provides a resolvent estimate). To justify the latter, we find simple L^p-potentials with $p > 1$ for which (22.2) holds, with the decay rate faster than any power of $1/|\lambda|$, in a region Ω determined by (22.81), which essentially coincides with the set appearing in [13, Thm. 5]. Thus the very natural reason for the appearance of such Ω is provided.

The existence of this region Ω, where the spectrum of H_V is extremely unstable with respect to further, even tiny, perturbations, is a crucial difference with respect to the L^1-potentials. In the latter case, the resolvent estimate preventing that the resolvent of H_V explodes for large λ's again follows from the Birman-Schwinger estimate, see [2].

Higher dimensions

The results and methods of this paper are essentially one-dimensional. Nonetheless, the results have consequences for multi-dimensional Schrödinger operators with (at least local) symmetries and their not too strong perturbations. The pseudomodes in $L^2(\mathbb{R})$ from Section 22.3 are obviously applicable for problems allowing for the separation of variables in Cartesian coordinates, while the pseudomodes in $L^2(\mathbb{R}_+)$ from Section 22.5 are applicable for radially symmetric problems. Finally, the pseudomodes from Example 22.11 arising due to the strongly singular potential at 0, namely

$$V(r) := \frac{c}{r^2} + \frac{i}{r^\alpha}\,, \qquad c \in \mathbb{R}, \quad \alpha > 2, \quad r > 0\,, \tag{22.6}$$

localise in a vicinity of 0 and so are applicable for multi-dimensional potentials with a local radial singularity of the type (22.6). Unlike in one dimension, these pseudomodes do not show the optimality of region Ω in Laptev-Safronov multi-dimensional eigenvalue bounds since the condition $\alpha > 2$ cannot be satisfied for $V \in L^p(\mathbb{R}^d)$ with $p \geq d/2$ (or $p > 1$ for $d = 2$).

Organisation of the paper

In Section 22.2 we outline our strategy to construct the pseudomodes and settle a number of important prerequisites for the subsequent applications. Section 22.3 is devoted to large positive pseudoeigenvalues, while the case of general complex regions is treated only in Section 22.5; these two sections are concerned with sufficiently regular potentials (at least continuous). Large positive pseudoeigenvalues for discontinuous and singular potentials are dealt with in the intermediate Section 22.4.

Notations

Let us fix some notations employed throughout the paper. We use the following conventions for number sets, $\mathbb{N} := \{1, 2, \dots\}$, $\mathbb{N}_0 := \mathbb{N} \cup \{0\}$, $\mathbb{R}_+ := (0, \infty)$ and $\mathbb{R}_- := (-\infty, 0)$. Given an interval $I \subset \mathbb{R}$, the norm of $L^p(I)$ is denoted by $\|\cdot\|_{L^p(I)}$. If $I = \mathbb{R}$, we abbreviate $\|\cdot\|_p := \|\cdot\|_{L^p(\mathbb{R})}$ and $\|\cdot\| := \|\cdot\|_2$. The L^p spaces with a weight are denoted by

$$L^p_\alpha(I) := \{f \text{ measurable} : \langle x\rangle^\alpha f(x) \in L^p(I)\}, \quad \alpha \in \mathbb{R}\,, \tag{22.7}$$

where $\langle x\rangle := (1 + x^2)^{\frac{1}{2}}$. For an "integer interval" we use the double brackets, $[[m, n]] := [m, n] \cap \mathbb{Z}$. To avoid using many irrelevant constants, we employ the convention that $a \lesssim b$ if there is a constant $C > 0$, independent of λ and x (or any other relevant parameter), such that $a \leq Cb$; the convention for $\gtrsim$ is analogous. By $a \approx b$ it is meant that $a \lesssim b$ and $a \gtrsim b$.

22.2 Preliminaries

A standing hypothesis of this paper is that the complex-valued potential V satisfies the local square-integrability condition $V \in L^2_{\mathrm{loc}}(\mathbb{R})$. We understand the Schrödinger operator (22.8) as the maximal operator generated by the differential expression, *i.e.*,

$$\begin{aligned} H_V f &:= -f'' + Vf\,, \\ \mathsf{D}(H_V) &:= \{f \in L^2(\mathbb{R}) : -f'' + Vf \in L^2(\mathbb{R})\}\,. \end{aligned} \tag{22.8}$$

If $\Re V$ is bounded from below, Kato's theorem (*cf* [8, Sec. VII.2.2]) yields that H_V is m-accretive and, moreover, $C_0^\infty(\mathbb{R})$ is a core of H_V. The m-accretivity ensures that (22.8) is well defined as a closed operator with non-empty resolvent set. The latter properties of H_V are valid also in the non-accretive case under alternative assumptions on V, see [10]. For the pseudomode constructions performed in the present paper, however, not even the closedness of H_V is necessary.

22.2.1 The JWKB Ansatz

Our construction of pseudomodes is based on the Liouville-Green approximation (also known as the JWKB method). If V were constant, *i.e.* $V(x) = V_0$ for all $x \in \mathbb{R}$, exact solutions of the differential equation $-g'' + V_0 g = \lambda g$ would be given by

$$e^{\pm i \int_0^x \sqrt{\lambda - V_0}\,\mathrm{d}t}\,. \tag{22.9}$$

We shall be particularly interested in the limit $\lambda \to +\infty$ and consistently consider the *principal branch* of the square root. More generally, we always restrict to

$$\lambda \in \mathbb{C} \setminus (-\infty, 0)\,. \tag{22.10}$$

For a variable potential V, we still take (22.9) with V_0 replaced by V and with the minus sign (due to assumptions on the signs of $\Im V$, see (22.28)) as a basic Ansatz to get the approximate solutions (22.2). Nonetheless, usually more terms will be needed for unbounded potentials or when V is sufficiently regular and more information on the decay rates in (22.2) are sought. In general, we therefore take

$$g(x) := \exp\left(-\sum_{k=-1}^{n-1} \lambda^{-\frac{k}{2}} \psi_k(x)\right), \tag{22.11}$$

where functions ψ_k are to be determined. Not surprisingly, ψ_{-1} will turn out to be given by $\psi_{-1}(x) := i\lambda^{-1/2} \int_0^x \sqrt{\lambda - V(t)}\,\mathrm{d}t$. As we will show in examples in Section 22.3.4, most of interesting potentials can be treated already with the expansion (22.11) up to $n = 2$.

22.2.2 The cut-off

To obtain admissible pseudomodes, it is important to employ a λ-dependent cut-off of the JWKB Ansatz (22.11). To this aim, we consider a function $\xi : \mathbb{R} \to \mathbb{R}$ satisfying the following properties:

$$\begin{aligned} &\xi \in C_0^\infty(\mathbb{R}), \quad 0 \leq \xi \leq 1, \\ &\forall x \in (-\delta_- + \Delta_-, \delta_+ - \Delta_+), \quad \xi(x) = 1, \\ &\forall x \notin (-\delta_-, \delta_+), \quad \xi(x) = 0; \end{aligned} \tag{22.12}$$

the λ-dependent positive numbers $\delta_\pm = \delta_\pm(\lambda)$ and $\Delta_\pm = \Delta_\pm(\lambda) < \delta_\pm$ will be determined later. Notice that ξ can be selected in such a way that

$$\|\xi^{(j)}\|_{L^\infty(\mathbb{R}_\pm)} \lesssim \Delta_\pm^{-j}, \quad j = 1, 2. \tag{22.13}$$

To simplify notations, we also define intervals

$$\begin{aligned} \mathcal{J} &:= (-\delta_-, \delta_+), & \mathcal{J}_\pm &:= \{x \in \mathbb{R}_\pm \,:\, |x| < \delta_\pm\}, \\ \mathcal{J}' &:= (-\delta_- + \Delta_-, \delta_+ - \Delta_+), & \mathcal{J}'_\pm &:= \{x \in \mathbb{R}_\pm \,:\, |x| < \delta_\pm - \Delta_\pm\}. \end{aligned} \tag{22.14}$$

Our Ansatz for a general potential V then reads

$$f := \xi\, g. \tag{22.15}$$

where g is defined in (22.11) and the index $n \in \mathbb{N}_0$ will be chosen according to the smoothness of V.

22.2.3 The strategy

Let us informally describe the strategy. Recalling (22.11), we have

$$\begin{aligned} -f'' + (V - \lambda) f &= -(\xi\, g)'' + (V - \lambda)\xi\, g \\ &= -\xi'' g - 2\xi' g' + \xi[-g'' + (V - \lambda) g]. \end{aligned} \tag{22.16}$$

When $n = 0$, the appearing terms read

$$g' = -i\sqrt{\lambda - V} g, \qquad -g'' + (V - \lambda) g = \frac{-iV'}{\sqrt{\lambda - V}}\, g\,, \tag{22.17}$$

which already suggests what needs to be done. First, V must be sufficiently regular so that $f \in \mathsf{D}(H_V)$; in fact, the more terms in (22.11) are taken, the more regular V is needed. Second, functions ψ_k in (22.11) and the cut-off ξ must be selected in such a way that the L^2-norm of the third term on the second line of (22.16) is as small as possible when λ is large. Third, the assumption on the sign of $\Im V$, see (22.28), implies that $|g|$ decays exponentially, see Lemma 22.4, and so the terms with ξ' and ξ'' are expected to be small; nevertheless, an appropriate restriction of $\delta_\pm$, $\Delta_\pm$ must be given.

Since our goal is to deal with potentials of low regularity, the construction consists of more steps. First we deal with sufficiently regular potentials V, later we add a singular term W and follow various possible strategies how to treat it, see Section 22.4.

22.2.4 The expansion

For g given in (22.11), we have

$$\begin{aligned} -g'' + (V - \lambda) g &= \left(\sum_{k=-1}^{n-1} \lambda^{-\frac{k}{2}} \psi_k''\right) g - \left(\sum_{k=-1}^{n-1} \lambda^{-\frac{k}{2}} \psi_k'\right)^2 g + (V - \lambda) g \\ &=: \left(\sum_{k=-2}^{2(n-1)} \lambda^{-\frac{k}{2}} \phi_{k+1}\right) g, \qquad n \in \mathbb{N}. \end{aligned} \tag{22.18}$$

Here the functions ϕ_k with $k \in [[-1, 2n-1]]$ are naturally defined after grouping together the terms with the same power of λ on the right hand side of the first line in (22.18), with the exception of V which we include in the leading order term:

$$\begin{aligned} &(k = -2) && \lambda^1 : && -(\psi_{-1}')^2 + \frac{V - \lambda}{\lambda} =: \phi_{-1}, \\ &(k = -1) && \lambda^{\frac{1}{2}} : && \psi_{-1}'' - 2\psi_{-1}'\psi_0' =: \phi_0, \\ &(k = 0) && \lambda^0 : && \psi_0'' - 2\psi_{-1}'\psi_1' - (\psi_0')^2 =: \phi_1, \\ &(k = 1) && \lambda^{-\frac{1}{2}} : && \psi_1'' - 2\psi_{-1}'\psi_2' - 2\psi_0'\psi_1' =: \phi_2, \\ &\dots \end{aligned} \tag{22.19}$$

For $-1 \le k \le 2(n-1)$, the formulae can be written concisely as

$$\psi_k'' - \sum_{\alpha+\beta=k} \psi_\alpha' \psi_\beta' = \phi_{k+1}\,, \tag{22.20}$$

with the convention that $\psi_\alpha = 0$ whenever $\alpha \geq n$ or $\alpha \leq -2$.

For the given $n \in \mathbb{N}$, we have $n+1$ functions $\psi_{-1}, \dots, \psi_{n-1}$ and $2n+1$ functions $\phi_{-1}, \dots, \phi_{2n-1}$. The strategy is to require that the first $n+1$ functions $\phi_{-1}, \dots, \phi_{n-1}$ are equal to zero, which determines all available ψ_k. Using (22.20), this leads to a system of $n+1$ first-order differential equations that the functions $\psi_{-1}, \dots, \psi_{n-1}$ must satisfy:

$$\begin{aligned} \psi_{-1}' &= i\lambda^{-\frac{1}{2}}(\lambda - V)^{\frac{1}{2}}\,, \\ \psi_{k+1}' &= \frac{1}{2\psi_{-1}'}\left(\psi_k'' - \sum_{\substack{\alpha+\beta=k \\ \alpha,\beta\neq -1}} \psi_\alpha' \psi_\beta'\right), \qquad k \in [[-1, n-2]]\,, \end{aligned} \tag{22.21}$$

with the convention as above that $\psi_\alpha = 0$ whenever $\alpha \geq n$ or $\alpha \leq -2$. Here and in the sequel λ is, in addition to (22.10), assumed to be such that $\lambda - V(x) \in \mathbb{C} \setminus (-\infty, 0)$ for all $x \in \mathbb{R}$. Recall that the principal branch of the square root is considered in this paper.

Notice that we had a freedom in the choice of sign in the definition of ψ_{-1}' to make $\phi_{-1} = 0$, see (22.19). Our choice made in (22.21) will be consistently followed in this paper.

Finally, with this choice of functions ψ_k we get

$$-g'' + (V - \lambda)g = \left(\sum_{k=n-1}^{2(n-1)} \lambda^{-\frac{k}{2}} \phi_{k+1}\right) g =: r_n\, g, \qquad n \in \mathbb{N}. \tag{22.22}$$

The essential point for estimating the resulting term is the understanding of the structure of functions ψ_k' and remainders r_n, which is the content of the following lemmata. The proof is based on a straightforward but rather lengthy induction argument.

Lemma 22.1. *Let $n \in \mathbb{N}_0$, $V \in W^{n+1,2}_{\mathrm{loc}}(\mathbb{R})$ and functions $\{\psi_k'\}_{k\in[[-1,n-1]]}$ be determined by (22.21). Then*

$$\psi_k^{(m)} = \frac{\lambda^{\frac{k}{2}}}{(\lambda - V)^{\frac{k}{2}}} \sum_{j=0}^{k+m} \frac{T_j^{k+m,k+m+1-j}}{(\lambda - V)^j}, \quad m \in [[1, n+1-k]], \tag{22.23}$$

where (with some $c_\alpha \in \mathbb{C}$)

$$\begin{aligned} T_j^{r,s} &:= \sum_{\alpha \in \mathcal{J}_j^{r,s}} c_\alpha (V^{(1)})^{\alpha_1} (V^{(2)})^{\alpha_2} \dots (V^{(s)})^{\alpha_s}, \\ \mathcal{J}_j^{r,s} &:= \left\{ \alpha \in \mathbb{N}_0^s \,:\, \sum_{i=1}^{s} i\alpha_i = r \;\&\; \sum_{i=1}^{s} \alpha_i = j \right\}. \end{aligned} \tag{22.24}$$

Moreover, if $r \geq 1$, then $\mathcal{J}_0^{r,r+1} = \emptyset$.

Lemma 22.2. *Let $n \in \mathbb{N}_0$, $V \in W^{n+1,2}_{\mathrm{loc}}(\mathbb{R})$ and functions $\{\psi_k'\}_{k\in[[-1,n-1]]}$ be determined by (22.21), $\{\phi_k\}_{k\in[[-1,2n-1]]}$ be as in (22.20) and r_n as in (22.22). Then*

$$|r_n| \lesssim \frac{|V^{(n+1)}|}{|\lambda - V|^{\frac{n+1}{2}}} + \sum_{k=0}^{n-1} \frac{1}{|\lambda - V|^{\frac{n-1+k}{2}}} \sum_{l=2}^{n+1+k} \frac{|T_l^{n+1+k,n}|}{|\lambda - V|^l}, \tag{22.25}$$

where $T_j^{r,s}$ are as in (22.24).

As an illustration for the expansions above with $n = 0, 1, 2$ we list functions ψ_k':

$$\begin{aligned} &(n=0) \qquad \psi_{-1}' = i\frac{(\lambda - V)^{\frac{1}{2}}}{\lambda^{\frac{1}{2}}}, \\ &(n=1) \qquad \psi_0' = -\frac{1}{4}\frac{V'}{\lambda - V}, \\ &(n=2) \qquad \psi_1' = \frac{i}{2}\frac{\lambda^{\frac{1}{2}}}{(\lambda - V)^{\frac{1}{2}}}\left(\frac{1}{4}\frac{V''}{\lambda - V} + \frac{5}{16}\frac{V'^2}{(\lambda - V)^2}\right), \end{aligned} \tag{22.26}$$

together with the remainders r_n on the right of (22.22):

$$
\begin{aligned}
r_0 &= -\frac{i}{2}\frac{V'}{(\lambda-V)^{\frac{1}{2}}},\\
r_1 &= -\frac{1}{4}\frac{V''}{\lambda-V} - \frac{5}{16}\frac{V'^2}{(\lambda-V)^2},\\
r_2 &= \frac{i}{8}\frac{1}{(\lambda-V)^{\frac{1}{2}}}\left(\frac{V'''}{(\lambda-V)} + \frac{9}{2}\frac{V'V''}{(\lambda-V)^2} + \frac{15}{4}\frac{V'^3}{(\lambda-V)^3}\right)\\
&\quad + \frac{1}{64}\frac{1}{(\lambda-V)}\left(\frac{V''^2}{(\lambda-V)^2} + \frac{5}{2}\frac{V'^2V''}{(\lambda-V)^3} + \frac{25}{16}\frac{V'^4}{(\lambda-V)^4}\right).
\end{aligned}
\tag{22.27}
$$

22.3 Pseudomodes for $\lambda \to +\infty$

In this section, unless otherwise stated, we always assume that λ is *positive* and typically very large.

22.3.1 Admissible class of potentials

We proceed under the following hypothesis about the (possibly unbounded) potential V.

Assumption 22.1. Let $N \in \mathbb{N}$ and let $V \in W^{N,\infty}_{\mathrm{loc}}(\mathbb{R})$ satisfy the following conditions:

a) $\Im V$ has a different asymptotic behaviour at $\pm\infty$:

$$
\limsup_{x\to-\infty} \Im V(x) < 0, \qquad \liminf_{x\to+\infty} \Im V(x) > 0;
\tag{22.28}
$$

b) derivatives of V are controlled by V: $\exists \nu_\pm \in \mathbb{R}$, $\forall m \in [[1, N]]$,

$$
\begin{aligned}
|\Im V^{(m)}(x)| &= \mathcal{O}\left(|\Im V(x)|\langle x\rangle^{m\nu_\pm}\right), \quad x \to \pm\infty,\\
|V^{(m)}(x)| &= \mathcal{O}\left(|V(x)|\langle x\rangle^{m\nu_\pm}\right), \quad x \to \pm\infty;
\end{aligned}
\tag{22.29}
$$

c) $\Im V$ is sufficiently large:

i) if V is unbounded at $\pm\infty$, then suppose that: $\exists \varepsilon_1 > 0$,

$$
\langle x\rangle^{4(\nu_\pm+\varepsilon_1)+2}(\langle x\rangle^{4\nu_\pm+2} + |\Re V(x)|) = \mathcal{O}\left(|\Im V(x)|^2\right), \quad x \to \pm\infty;
\tag{22.30}
$$

ii) if V is bounded at $\pm\infty$, then suppose that $\nu_\pm < 1$, where $\nu_\pm$ are the numbers from (22.29).

Several comments on the assumption are in place. First of all, notice that V is necessarily continuous due to $V \in W^{1,\infty}_{\mathrm{loc}}(\mathbb{R})$.

The condition (22.28) ensures that the operator (22.1) is "significantly non-self-adjoint". More precisely, H_V is not normal as a consequence of (22.28), the normality being equivalent to the condition that $\Im V$ is constant. Furthermore, hypothesis (22.28) ensures that the pseudomode g from (22.11) is exponentially decaying. The correct sign for the decay can be seen (if the shape of g is determined mainly by ψ_{-1}) by employing (22.28) and the complex square root formula

$$
\begin{aligned}
\Re\left(\lambda^{\frac{1}{2}}\psi'_{-1}\right) &= -\Im(\lambda-V)^{\frac{1}{2}}\\
&= \frac{1}{2^{\frac{1}{2}}}\frac{\Im V}{\left([(\lambda-\Re V)^2 + (\Im V)^2]^{\frac{1}{2}} + (\lambda-\Re V)\right)^{\frac{1}{2}}},
\end{aligned}
\tag{22.31}
$$

valid for all positive λ satisfying in addition the requirement $\lambda - V(x) \in \mathbb{C}\setminus(-\infty,0)$ for all $x \in \mathbb{R}$. The remaining two intertwined conditions guarantee that the exponential decay of g is not spoiled by too large $\Re V$ or too wild behaviour of the derivatives of V.

The condition (22.29) restricts the growth and oscillations of V, nonetheless, it is still quite flexible as *e.g.* $V(x) := \pm ie^{x^2}$ for $x \to \pm\infty$ is covered. Notice that Gronwall's inequality implies that (with some $M > 0$)

$$
\forall x \geq 0, \quad |V(x)| \lesssim \begin{cases} e^{Mx^{1+\nu_+}}, & \nu_+ > -1,\\ \langle x\rangle^M, & \nu_+ = -1,\\ 1, & \nu_+ < -1; \end{cases}
\tag{22.32}
$$

an analogous estimate holds also for $x \leq 0$.

If V is bounded, we do not require that the derivatives of V are bounded in general, thus *e.g.* rapidly oscillating potentials are allowed. In such cases, the estimate from Gronwall's inequality becomes very crude.

The condition (22.29) also implies that for $\nu_+ \geq -1$ and all sufficiently large $x > 0$ and every $|\Delta| \leq x^{-\nu_+}/4$, we have

$$\frac{|\Im V(x+2\Delta)|}{|\Im V(x)|} \approx 1. \tag{22.33}$$

Indeed, for $\nu_+ > -1$,

$$\begin{aligned}\left|\log \frac{|\Im V(x+2\Delta)|}{|\Im V(x)|}\right| &= \left|\int_x^{x+2\Delta} \frac{\Im V'(t)}{\Im V(t)}\,\mathrm{d}t\right| \lesssim \left||x+2\Delta|^{\nu_++1} - |x|^{\nu_++1}\right| \\ &\lesssim x^{\nu_+}|\Delta| + \mathcal{O}(|\Delta|^2 x^{\nu_+-1}),\end{aligned} \tag{22.34}$$

and similarly for $\nu_+ = -1$. The conclusion (22.33) is clearly valid also for bounded V as we require (22.28).

22.3.2 Localisation of the pseudomode and cut-off

To estimate $|g|$ we first show that under Assumption 22.1 the function $\int_0^x [\lambda^{\frac{1}{2}}\psi_{-1}'(t) + \psi_0'(t)]\,\mathrm{d}t$ in the expansion (22.11) dominates over the other terms with $k \geq 1$. Thus estimates simplify significantly even for many terms in (22.11). Already at this step, it is important to employ a suitable cut-off. Namely, for every $\lambda > 0$ we define:

$$\begin{aligned}\delta_\pm &:= \begin{cases} \inf\left\{\delta \geq 0 \,:\, \dfrac{|\Im V(\pm\delta)|^2}{\langle\delta\rangle^{4\nu_\pm+2\varepsilon_1+2}} = \lambda\right\} & \text{if } V \text{ is unbounded at } \pm\infty, \\ \lambda^{\frac{1+\varepsilon_2}{2}} \quad \text{with} \quad 0 < \varepsilon_2 < 1-\nu_\pm & \text{if } V \text{ is bounded at } \pm\infty, \end{cases} \\ \Delta_\pm &:= \frac{1}{4}\begin{cases} \delta_\pm^{-\nu_\pm} & \text{if } V \text{ is unbounded at } \pm\infty, \\ \delta_\pm & \text{if } V \text{ is bounded at } \pm\infty. \end{cases}\end{aligned} \tag{22.35}$$

Remark 22.1 (Properties of $\delta_\pm$ and $\Delta_\pm$)**.** The following hold.

i) The infimum can be infinite ($\inf \varnothing = +\infty$), however, for all sufficiently large $\lambda > 0$, the numbers $\delta_\pm$ are finite and

$$\lim_{\lambda\to+\infty} \delta_\pm = +\infty; \tag{22.36}$$

ii) $\Delta_\pm$ are so small that the values of $\Im V(x)$ are comparable if $|x - \delta_\pm| \leq 2\Delta_\pm$;

iii) for all sufficiently large $\lambda > 0$,

$$\forall x \in \mathcal{J}, \quad |\lambda - V(x)| \approx \lambda. \tag{22.37}$$

Proof. All the three properties are obvious for bounded V. We further assume that V is unbounded at $+\infty$ and prove the claims; the case of V unbounded at $-\infty$ is analogous.

i) It follows from the assumption (22.30) that for all sufficiently large $\delta > 0$

$$\frac{|\Im V(\delta)|^2}{\langle\delta\rangle^{4\nu_++2\varepsilon_1+2}} \gtrsim \langle\delta\rangle^{2\varepsilon_1}, \tag{22.38}$$

thus for all

$$\lambda > \min_{\delta\geq 0} \frac{|\Im V(\delta)|^2}{\langle\delta\rangle^{4\nu_++2\varepsilon_1+2}} \tag{22.39}$$

the number δ_+ is finite. Since $\Im V$ is continuous, (22.36) follows.

ii) See (22.33).

iii) From (22.30), we obtain that for all $x > x_0$ with x_0 sufficiently large,

$$|\Im V(x)| \lesssim \frac{|\Im V(x)|^2}{\langle x\rangle^{4\nu_++2\varepsilon_1+2}}, \qquad |\Re V(x)| \lesssim \frac{|\Im V(x)|^2}{\langle x\rangle^{4\nu_++4\varepsilon_1+2}}; \tag{22.40}$$

thus we may assume that x_0 is chosen so large that for all $x > x_0$, we have

$$|\Re V(x)| \leq \frac{1}{2}\frac{|\Im V(x)|^2}{\langle x\rangle^{4\nu_++2\varepsilon_1+2}}. \tag{22.41}$$

Thus, using (22.35), already proved i) and the continuity of V, we can select sufficiently large $\lambda_0 > 0$ such that for all $\lambda > \lambda_0$ and all $x \in [0, \delta_+]$, we have

$$|\Im V(x)| \lesssim \lambda, \qquad |\Re V(x)| \leq \frac{\lambda}{2}. \tag{22.42}$$

Hence (22.37) follows. □

Remark 22.2 (More on the assumption on $\Re V$)**.** The restriction on $\Re V$ made in (22.30) arises in a very natural way. As an illustration, let us consider the potential $V(x) := |x|^\beta + i\,\mathrm{sgn}(x)\,|x|^\gamma$ with positive powers β, γ. In this case we can take $\nu_\pm := -1$ to satisfy hypothesis (22.29) and assumption (22.30) imposes the relationship $\beta - 2 + 4\varepsilon_1 \leq 2\gamma$. Choosing on the contrary $\beta > 2\gamma + 2$ so that (22.30) is violated, the dominant part in the expansion (22.11), which is given by $\Re\left(\lambda^{\frac{1}{2}}\psi'_{-1}\right)$ as we show later, becomes (uniformly in λ) *integrable* in $x \in \mathbb{R}$. Indeed, with the substitution $t = \lambda^{1/\beta}s$ and by straightforward estimates,

$$\int_0^{\delta_+} \left|\Re\left(\lambda^{\frac{1}{2}}\psi'_{-1}(t)\right)\right| \,\mathrm{d}t \lesssim \lambda^{\frac{2+2\gamma-\beta}{2\beta}} \int_0^\infty \frac{s^\gamma}{|1 - s^\beta|^{\frac{1}{2}}} \,\mathrm{d}s = o(1), \quad \lambda \to +\infty. \tag{22.43}$$

Moreover, notice that by taking a larger δ, so that it is possible that $\Re V(x) \geq \lambda$, we get into troubles with the decay of $|r_n|$ for which the estimate $|\Re V - \lambda| \gtrsim \lambda$ is essential.

Using the properties of $\delta_\pm$ and $\Delta_\pm$, we obtain the following estimates.

Lemma 22.3. *Let Assumption 22.1 hold, let $0 \leq n \leq N$ and $\{\psi'_k\}_{k \in [[-1, n-1]]}$ be determined by (22.21) and let $\delta_\pm$ be as in (22.35). Then for all sufficiently large $\lambda > 0$*

$$\forall x \in \mathcal{J}, \qquad \lambda^{\frac{1}{2}}\Re\psi'_{-1}(x) \approx \lambda^{-\frac{1}{2}}\Im V(x), \tag{22.44}$$

and

$$\forall k \in [[0, n-1]], \quad \forall x \in \mathcal{J}_\pm, \qquad \lambda^{-\frac{k}{2}}|\psi'_k(x)| \lesssim \frac{|V(x)|\langle x\rangle^{(k+1)\nu_\pm}}{\lambda^{\frac{k}{2}+1}}. \tag{22.45}$$

Proof. The estimate (22.44) follows immediately from (22.31) using (22.37) and (22.42). The rest is based on Lemma 22.1 and assumptions (22.29), (22.30).

For $k \geq 0$, Lemma 22.1 yields

$$\begin{aligned} \lambda^{-\frac{k}{2}}|\psi'_k| &\leq \frac{1}{|\lambda - V|^{\frac{k}{2}}} \sum_{j=1}^{k+1} \frac{|T_j^{k+1,k+2-j}|}{|\lambda - V|^j} \\ &\lesssim \frac{1}{|\lambda - V|^{\frac{k}{2}}} \sum_{j=1}^{k+1} \frac{\sum_{\alpha \in \mathcal{J}_j^{k+1,k+2-j}} |V'|^{\alpha_1}|V''|^{\alpha_2} \ldots |V^{(k+2-j)}|^{\alpha_{k+2-j}}}{|\lambda - V|^j}. \end{aligned} \tag{22.46}$$

Notice that the highest derivative of V that appears is $V^{(n)}$ and that the product of $|V^{(i)}|$ consists always of j factors (counting with powers) since $\sum_{i=1}^{k+2-j} \alpha_i = j$; see (22.24). Thus all appearing derivatives of V are continuous and the assumption (22.29) with $\sum_{i=1}^{k+2-j} i\alpha_i = k+1$ from (22.24) yields that for all sufficiently large $x > 0$

$$\lambda^{-\frac{k}{2}}|\psi'_k(x)| \lesssim \frac{\langle x\rangle^{(k+1)\nu_+}}{|\lambda - V(x)|^{\frac{k}{2}}} \sum_{j=1}^{k+1} \frac{|V(x)|^j}{|\lambda - V(x)|^j} \lesssim \frac{|V(x)|\langle x\rangle^{(k+1)\nu_+}}{\lambda^{\frac{k}{2}+1}}; \tag{22.47}$$

in the last step we have used (22.37). For small $x > 0$, the estimate (22.45) follows immediately from (22.46) and the continuity of the derivatives of V. For $x < 0$, the estimate is analogous. □

Localising the Ansatz (22.11) on the interval $\mathcal{J}$, the preceding lemma shows that the shape of g is determined mainly by ψ_{-1} and ψ_0. More specifically, given the derivatives ψ'_k from (22.21), henceforth we choose the primitive functions ψ_k by fixing the integration constant by the requirement

$$\psi_k(0) := 0\,, \qquad k \in [[-1, n-1]]\,. \tag{22.48}$$

With this standing convention, we have the following two-sided bounds.

Lemma 22.4. *Let Assumption 22.1 hold, g be as in* (22.11) *with* $\{\psi_k'\}_{k\in[[-1,n-1]]}$, $0 \leq n \leq N$, *determined by* (22.21) *and let $\delta_\pm$ be as in* (22.35). *Then there exist $c_1, c_2 > 0$ such that for all sufficiently large $\lambda > 0$ and all $x \in \mathcal{J}$ we have*

$$\exp\left(-\frac{c_1}{\lambda^{\frac{1}{2}}}\int_0^{|x|}|\Im V(t)|\,\mathrm{d}t\right) \lesssim |g(x)| \lesssim \exp\left(-\frac{c_2}{\lambda^{\frac{1}{2}}}\int_0^{|x|}|\Im V(t)|\,\mathrm{d}t\right). \tag{22.49}$$

Proof. Notice that the formula (22.26) for ψ_0' is exceptional since it can be easily integrated, hence

$$g(x) = \frac{[\lambda - V(0)]^{\frac{1}{4}}}{[\lambda - V(x)]^{\frac{1}{4}}}\exp\left(-\sum_{\substack{k=-1\\k\neq 0}}^{n-1}\lambda^{-\frac{k}{2}}\int_0^x \psi_k'(t)\,\mathrm{d}t\right). \tag{22.50}$$

From (22.37) we get

$$\forall x \in \mathcal{J}, \qquad \left|\frac{\lambda - V(0)}{\lambda - V(x)}\right| \approx 1. \tag{22.51}$$

We continue with estimates for $x > 0$, the other case is analogous. For any $x_0 > 0$ fixed, we have from Lemma 22.3 that

$$\left|\Re\sum_{k=-1}^{n-1}\lambda^{-\frac{k}{2}}\int_0^{x_0}\psi_k'(t)\,\mathrm{d}t\right| \lesssim \lambda^{-\frac{1}{2}}. \tag{22.52}$$

The remaining estimate for $x > x_0$ follows from (22.45), (22.35) and assumption (22.30), namely

$$\Re\sum_{\substack{k=-1\\k\neq 0}}^{n-1}\lambda^{-\frac{k}{2}}\int_{x_0}^x \psi_k'(t)\,\mathrm{d}t = \int_{x_0}^x \lambda^{\frac{1}{2}}\Re\psi_{-1}'(t)\,[1 + S(t)]\,\mathrm{d}t,. \tag{22.53}$$

where

$$|S(t)| \lesssim \begin{cases} \lambda^{-\frac{1}{2}} & \text{if } V \text{ is unbounded},\\ \lambda^{-\frac{1}{2}} & \text{if } V \text{ is bounded and } \nu_+ < 0,\\ \lambda^{-\frac{1-(1+\varepsilon_2)\nu_+}{2}} & \text{if } V \text{ is bounded and } \nu_+ \geq 0. \end{cases} \tag{22.54}$$

Indeed, in the first case Lemma 22.3, assumption (22.30), (22.37) and (22.44) give

$$\frac{\lambda^{\frac{k}{2}}|\psi_k'(x)|}{\lambda^{\frac{1}{2}}|\Re\psi_{-1}'(x)|} \lesssim \frac{\langle x\rangle^{(k+1)\nu_\pm}}{\lambda^{\frac{k-1}{2}}|\Im V(x)|} \lesssim \frac{1}{\langle x\rangle^{\frac{k+1}{2}(\varepsilon_1+1)}\lambda^{\frac{k+1}{4}}}; \tag{22.55}$$

the other cases can be verified similarly.

Hence using (22.44) we get

$$\Re\sum_{\substack{k=-1\\k\neq 0}}^{n-1}\lambda^{-\frac{k}{2}}\int_{x_0}^x \psi_k'(t)\,\mathrm{d}t \approx \lambda^{-\frac{1}{2}}\int_{x_0}^x \Im V(t)\,\mathrm{d}t. \tag{22.56}$$

Putting all estimates from above together, we obtain (22.49). □

The following proposition ensures that the terms in (22.16) containing derivatives of the cut-off function are negligible in a sense.

Proposition 22.1. *Let Assumption 22.1 hold, g be as in* (22.11) *with* $\{\psi_k'\}_{k\in[[-1,n-1]]}$, $0 \leq n \leq N$, *determined by* (22.21) *and ξ be as in* (22.12) *with $\delta_\pm$, $\Delta_\pm$ as in* (22.35). *Then*

$$\kappa(\lambda) := \frac{\|\xi'' g\| + \|\xi' g'\|}{\|\xi g\|} = o(1), \qquad \lambda \to +\infty. \tag{22.57}$$

More precisely, $\kappa(\lambda) = \kappa_-(\lambda) + \kappa_+(\lambda)$ where (with some $c > 0$)

$$\kappa_\pm(\lambda) = \begin{cases} \mathcal{O}\left(\exp(-c\,\delta_\pm^{\nu_\pm+1+\varepsilon_1})\right) & \textit{if } V \textit{ is unbounded at } \pm\infty,\\ \mathcal{O}\left(\exp\left(-c\,\lambda^{\frac{\varepsilon_2}{2}}\right)\right) & \textit{if } V \textit{ is bounded at } \pm\infty. \end{cases} \tag{22.58}$$

Proof. First notice that from (22.49) we have $\|\xi g\| \gtrsim 1$. The main step is to estimate $|g(x)|^2$ for $x \in \overline{\mathcal{J} \setminus \mathcal{J}'}$ where ξ' and ξ'' are supported. We give details only for $x > 0$; the other case is analogous.

We start with the case when V is unbounded at $+\infty$. Let $x_0 > 0$ be so large that $\Im V(x) > 0$ for all $x > x_0$. From the property (22.33) and selected size of Δ_+, see (22.35), we obtain for $x \in \mathcal{J}_+ \setminus \mathcal{J}'_+$ that

$$\int_{x_0}^{x} \Im V(t)\,\mathrm{d}t \geq \int_{\delta_+ - 2\Delta_+}^{x} \Im V(t)\,\mathrm{d}t \gtrsim \Delta_+ \Im V(\delta_+) \gtrsim \frac{\Im V(\delta_+)}{\delta_+^{\nu_+}}. \tag{22.59}$$

Thus using (22.35), we get

$$\begin{aligned} \lambda^{-\frac{1}{2}} \int_{0}^{x} \Im V(t)\,\mathrm{d}t &= \lambda^{-\frac{1}{2}} \int_{0}^{x_0} \Im V(t)\,\mathrm{d}t + \lambda^{-\frac{1}{2}} \int_{x_0}^{x} |\Im V(t)|\,\mathrm{d}t \\ &\gtrsim -\lambda^{-\frac{1}{2}} + \frac{\delta_+^{2\nu_+ + \varepsilon_1 + 1}}{\Im V(\delta_+)} \frac{\Im V(\delta_+)}{\delta_+^{\nu_+}} \gtrsim \delta_+^{\nu_+ + \varepsilon_1 + 1}. \end{aligned} \tag{22.60}$$

Hence it follows from (22.49) that (with some $c_3 > 0$)

$$\forall x \in \mathcal{J}_+ \setminus \mathcal{J}'_+, \qquad |g(x)| \lesssim \exp(-c_3 \delta_+^{\nu_+ + \varepsilon_1 + 1}). \tag{22.61}$$

Additional terms appearing in $\|\xi' g'\|_{L^2(\mathbb{R}_+)}$ can be estimated using (22.13), (22.35), (22.45), (22.37) and (22.32). In detail, for all $x \in \mathcal{J}_+ \setminus \mathcal{J}'_+$ we have (with some $c_4 > 0$)

$$\begin{aligned} |\xi'(x) g'(x)| &\lesssim \delta_+^{\nu_+} \sum_{k=-1}^{n} \lambda^{\frac{k}{2}} |\psi'_k(x)| \exp(-c_3 \delta_+^{\nu_+ + \varepsilon_1 + 1}) \\ &\lesssim \delta_+^{\nu_+} \left(\lambda^{\frac{1}{2}} + \sum_{k=0}^{n} \frac{\langle x \rangle^{(k+1)\nu_+}}{\lambda^{\frac{k}{2}}} \right) \exp(-c_3 \delta_+^{\nu_+ + \varepsilon_1 + 1}) \\ &\lesssim \delta_+^{\nu_+} \left(\frac{|V(\delta_+)|}{\delta_+^{2\nu_+ + \varepsilon_1 + 1}} + \delta_+^{(n+1)\nu_+} \right) \exp(-c_3 \delta_+^{\nu_+ + \varepsilon_1 + 1}) \\ &\lesssim \exp(-c_4 \delta_+^{\nu_+ + \varepsilon_1 + 1}). \end{aligned} \tag{22.62}$$

The term $\|\xi'' g\|_{L^2(\mathbb{R}_+)}$ is estimated similarly (and in fact more easily).

Putting everything together, we obtain (with some $c_5 > 0$)

$$\frac{\|\xi'' g\|_{L^2(\mathbb{R}_+)} + \|\xi' g'\|_{L^2(\mathbb{R}_+)}}{\|\xi g\|_{L^2(\mathbb{R}_+)}} \lesssim \exp(-c_5 \delta_+^{\nu_+ \varepsilon_1 + 1}). \tag{22.63}$$

If V is bounded at $+\infty$, the appropriate rate in (22.58) follows immediately from (22.49) and the selected size of $\delta_\pm$ and $\Delta_\pm$, see (22.35). ☐

22.3.3 Remainder estimate

Theorem 22.1. *Let Assumption 22.1 hold and set $n := N - 1$. Let g be as in (22.11) with $\{\psi'_k\}_{k \in [[-1, n-2]]}$ determined by (22.21), ξ be as in (22.12) with $\delta_\pm$, $\Delta_\pm$ as in (22.35) and f be as in (22.15). Then*

$$\frac{\|(H_V - \lambda) f\|}{\|f\|} = \kappa(\lambda) + \sigma^{(n)}(\lambda), \tag{22.64}$$

where κ is as in (22.58) and $\sigma^{(n)} = \sigma_-^{(n)} + \sigma_+^{(n)}$ with, as $\lambda \to +\infty$,

i) if V is unbounded at $\pm\infty$

$$\sigma_\pm^{(n)}(\lambda) = \begin{cases} \mathcal{O}(\lambda^{-\frac{n+1}{2}} \sup_{x \in \mathcal{J}_\pm} |V(x)| \langle x \rangle^{(n+1)\nu_\pm}), & \nu_\pm < 0, \\ \mathcal{O}\left(\delta_\pm^{(n+1)\nu_\pm} \lambda^{\frac{1-n}{2}} \right), & \nu_+ \geq 0, \end{cases} \tag{22.65}$$

ii) if V is bounded at $\pm\infty$

$$\sigma_\pm^{(n)}(\lambda) = \begin{cases} \mathcal{O}\left(\lambda^{-\frac{n+1}{2}} \right), & \nu_\pm < 0, \\ \mathcal{O}\left(\lambda^{-\frac{n+1}{2}(1 - (1+\varepsilon_2)\nu_\pm)} \right), & \nu_\pm \geq 0. \end{cases} \tag{22.66}$$

Proof. We employ the pseudomode construction for $n = N - 1$. The estimate of the remainder r_n, see (22.25), and the assumption (22.29) together with (22.37) and (22.42) yield that for $x > 0$ and V unbounded at $+\infty$ we have

$$|r_n(x)| \lesssim \begin{cases} |V(x)| \langle x \rangle^{(n+1)\nu_+} \lambda^{-\frac{n+1}{2}}, & \nu_+ < 0, \\ \delta_+^{(n+1)\nu_+} \lambda^{\frac{1-n}{2}}, & \nu_+ \geq 0, \end{cases} \tag{22.67}$$

and similarly for $x < 0$. Here the case $\nu_+ \geq 0$ also employs $\lambda \gtrsim \langle \delta_+ \rangle^{4\nu_+ + 2\varepsilon_1 + 2}$, which is a consequence of (22.30) and (22.35). If V is bounded at $\pm\infty$, the estimate of r_n follows straightforwardly from (22.25), assumptions (22.29), (22.30) and the choice of $\delta_\pm$ in (22.35). ☐

22.3.4 Examples

Example 22.1 (Polynomial-like potentials)**.** Consider V satisfying Assumption 22.1 with $\nu_- = \nu_+ = -1$ and having the form

$$V := P_\beta + iQ_\gamma\,, \tag{22.68}$$

where P_β and Q_γ are real-valued functions satisfying

$$\forall |x| \gtrsim 1, \qquad |P_\beta(x)| \lesssim \langle x \rangle^\beta, \qquad |Q_\gamma(x)| \approx \langle x \rangle^\gamma, \tag{22.69}$$

with some numbers $\beta \in \mathbb{R}$ and $\gamma \geq 0$. Typical examples of P_β and Q_γ are polynomials of degree β and γ, respectively. Notice that a necessary condition to satisfy (22.28) is $\gamma \geq 0$, while a sufficient which guarantees (22.30) additionally requires $\gamma > (\beta - 2)/2$. In particular for $\beta < 2$ (*i.e.* $|\Re V(x)|$ grows slower than x^2) even a bounded $\Im V$ fits.

We define the quantity

$$\omega := \max\{\beta, \gamma\} \geq 0 \tag{22.70}$$

and observe that $\omega = 0$ if, and only if, V is bounded. If ω is positive, then (22.35) yields

$$\delta = \delta_- = \delta_+ \approx \lambda^{\frac{1}{2(\gamma+1)} + \epsilon}, \tag{22.71}$$

where $\epsilon > 0$ can be made arbitrarily small by an appropriate choice of (small) $\varepsilon_1 > 0$. Hence the application of Theorem 22.1 yields (with $n := N - 1$)

$$\frac{\|(H_V - \lambda)f\|}{\|f\|} = \begin{cases} \mathcal{O}\left(\lambda^{-\frac{n+1}{2}}\right), & \omega \leq n+1, \\ \mathcal{O}\left(\lambda^{-\frac{n+1}{2} + \frac{\omega - n - 1}{2(\gamma+1)} + \epsilon(\omega - n - 1))}\right), & \omega > n+1, \end{cases} \tag{22.72}$$

as $\lambda \to +\infty$. Notice that the first case particularly involves bounded potentials (because $N \geq 1$) and that the decay rate in the second case improves by diminishing ϵ. It is also worth noticing that the restrictions on β and γ made above imply the uniform bounds

$$\frac{\omega - n - 1}{2(\gamma + 1)} < \begin{cases} 1/2 & \text{if} \quad \gamma \geq \beta\,, \\ 1 & \text{if} \quad \gamma < \beta\,, \end{cases} \tag{22.73}$$

which provides a rough estimate on the decay rate in the second case of (22.72).

Observe that the pseudomode with $n = 1$ (*i.e.* we require $N \geq 2$) is sufficient to treat all polynomial-like potentials. The pseudomode with $n = 0$ (*i.e.* $N \geq 1$) suffices for potentials growing not faster than linearly. Notice also that for smooth potentials ($N = \infty$) the obtained rate is faster than any power of λ^{-1}.

Example 22.2 (Exponential potentials)**.** Consider V satisfying Assumption 22.1 with $\nu_- = \nu_+ = 0$ and $N \geq 3$; a simple smooth choice is $V(x) := \cosh x + i \sinh x$. Since $|V(x)| \lesssim e^{|x|}$, see (22.32), we have for sufficiently large $\lambda > 0$ that

$$\delta = \delta_- = \delta_+ \approx \log \lambda. \tag{22.74}$$

Theorem 22.1 then gives

$$\frac{\|(H_V - \lambda)f\|}{\|f\|} = \mathcal{O}\left(\lambda^{\frac{2-N}{2}}\right), \tag{22.75}$$

thus exponential-type potentials can be treated with pseudomodes with $n = 2$.

Example 22.3 (Bounded oscillating potentials)**.** Consider two smooth potentials

$$V_1(x) := i \arctan x, \qquad V_2(x) := 2i \arctan x + i \sin\left(\langle x \rangle^{1+\mu}\right), \quad 0 < \mu < 1. \tag{22.76}$$

Clearly, $\nu_\pm = -2$ for V_1, however $\nu_\pm = \mu$ for V_2. Since both potentials are smooth, we can achieve an arbitrarily fast decay in (22.66) in both cases by taking N large, nevertheless, substantially more terms in the pseudomode construction must be taken in the second case if μ is close to 1.

22.3.5 Decaying potentials

Finally, we discuss a class of potentials that do not satisfy the basic assumption (22.28), but the method of the present section still enables one to construct the desired pseudomodes. Indeed, the inequalities (22.49) suggest that the assumption (22.28) can be relaxed basically to $\Im V \notin L^1(\mathbb{R})$ if $\Im V$ has an appropriate sign for $x \gtrsim 1$ and $x \lesssim 1$. Here we analyse the simplest examples, namely a class of smooth potentials with the asymptotic behaviour

$$V(x) := i\,\frac{\operatorname{sgn}(x)}{\langle x\rangle^{\gamma}}, \qquad |x| \gtrsim 1, \quad 0 < \gamma < 1. \tag{22.77}$$

Since the essential spectrum of H_V with this potential covers $[0, +\infty)$ and the numerical range of H_V is a shrinking neighbourhood of this set, we will consider $\lambda = a + ib$ with $a \to +\infty$ and $b \to 0+$.

The selection of a suitable $\delta_\pm$ for the cut-off is inspired by the estimate for $x \gtrsim 1$ (the case $x \lesssim -1$ and upper bounds are simpler)

$$\int_0^x \Re(\lambda^{\frac{1}{2}} \psi_{-1}'(t))\,\mathrm{d}t \gtrsim a^{-\frac{1}{2}} \int_0^x (\langle t\rangle^{-\gamma} - b)\,\mathrm{d}t \gtrsim \frac{x^{1-\gamma}[1 - (1-\gamma)bx^{\gamma}] - C}{a^{\frac{1}{2}}} \tag{22.78}$$

with some $C \geq 0$. Thus, requiring that the first term in the expansion (22.11) leads to an integrable exponential, sought restrictions on δ_+ read

$$a^{\frac{1}{2}} \delta_+^{\gamma-1} + b\delta_+^{\gamma} = o(1), \quad \lambda \to \infty; \tag{22.79}$$

δ_- can be selected similarly and we can take $\Delta_\pm := \delta_\pm/4$. It can be also checked that the other terms in the expansion are negligible. Since V is bounded, it is clear that the cut-off works and we indeed have a decay like in (22.57). Regarding the remainders r_n, by taking sufficiently many terms in the expansion, we obtain a decay in (22.2) that is faster than any power of a.

The set Ω where (22.2) holds can be obtained from (22.79); in detail, we need

$$b a^{\frac{\gamma}{2(1-\gamma)}} = o(1), \quad \lambda \to \infty. \tag{22.80}$$

Observing that $V \in L^p(\mathbb{R})$ if $p\gamma > 1$, we can further describe Ω by a condition essentially appearing in [13, Thm. 5]:

$$b^{p-1} = o(a^{-\frac{1}{2}}), \quad \lambda \to \infty. \tag{22.81}$$

22.4 Lower regularity

Our goal in this section is to treat potentials of lower regularity. The first possibility is a perturbative approach, *i.e.* we search for conditions on a possibly singular perturbation W guaranteeing that the pseudomodes constructed for a regular part V, thus ignoring W, still exhibit a decay in (22.2). The second option is to introduce a λ-dependent mollification W^ε of W with $\varepsilon = \varepsilon(\lambda)$ and perform the construction for $V + W^\varepsilon$; naturally the crucial point is to determine suitable dependence of the mollification on λ.

In both approaches we need eventually more precise information on the L^p-norms of pseudomodes. We make here additional assumptions on the growth of V; in fact we analyse in detail potentials with a polynomial growth, nonetheless, other cases may be treated similarly.

22.4.1 Weighted L^p-norms of pseudomodes

Lemma 22.5. *Let Assumption 22.1 hold, let f be as in* (22.15) *with $0 \leq n \leq N$. Then for all sufficiently large $\lambda > 0$ the following holds.*

i) If there is $\gamma \geq 0$ such that

$$\forall x \gtrsim 1, \quad |\Im V(x)| \lesssim |x|^{\gamma}, \qquad \text{or} \qquad \forall x \lesssim -1, \quad |\Im V(x)| \lesssim |x|^{\gamma}, \tag{22.82}$$

then

$$\|f\|_p \gtrsim \lambda^{\frac{1}{2p(\gamma+1)}}, \qquad 2 \leq p \leq \infty. \tag{22.83}$$

ii) If there are $\gamma_\pm \geq 0$ such that

$$|\Im V(x)| \gtrsim \begin{cases} |x|^{\gamma_+}, & x \gtrsim 1, \\ |x|^{\gamma_-}, & x \lesssim -1, \end{cases} \tag{22.84}$$

then

$$\|\langle x\rangle^{\alpha} f(x)\|_{L^p(\mathbb{R}_\pm)} \lesssim \lambda^{\frac{1+p\alpha}{2p(\gamma_\pm+1)}}, \qquad 2 \leq p \leq \infty, \quad \alpha \geq 0. \tag{22.85}$$

Proof. i) Suppose that the first inequality in (22.82) holds. From (22.49) we have (with some $C \geq 0$, $c > 0$)

$$\|f\|_p^p \gtrsim \int_C^{\delta_+-\Delta_+} e^{-pc\lambda^{-\frac{1}{2}}x^{\gamma+1}}\,\mathrm{d}x = \lambda^{\frac{1}{2(\gamma+1)}} \int_{C\lambda^{-\frac{1}{2(\gamma+1)}}}^{(\delta_+-\Delta_+)\lambda^{-\frac{1}{2(\gamma+1)}}} e^{-pcy^{\gamma+1}}\,\mathrm{d}y. \tag{22.86}$$

Thus it remains to verify that $(\delta_+ - \Delta_+)\lambda^{-\frac{1}{2(\gamma+1)}} \gtrsim 1$. The latter follows from (22.35). The case of bounded V is simple and in the unbounded case (necessarily with $\nu_+ \geq -1$, see (22.32)) we get from (22.82) and (22.35) that

$$\frac{\delta_+^{2(\gamma+1)}}{\lambda} \approx \frac{\delta_+^{2(\gamma+1)+4\nu_++2\varepsilon_1+2}}{|\Im V(\delta_+)|^2} \gtrsim \delta_+^{4\nu_++4+2\varepsilon_1} \gtrsim 1. \tag{22.87}$$

This proves (22.83) for $p \in [2, \infty)$ under the first of the assumptions in (22.82), the second alternative is treated similarly. The case $p = \infty$ is even simpler to show.

ii) For $x \geq 1$ we have $\langle x \rangle \approx x$, thus (22.49) and (22.84) yield (with some $C \geq 1$, $c > 0$)

$$\left(\int_0^C + \int_C^{\delta_+}\right) \langle x\rangle^{p\alpha} e^{-pc\lambda^{-\frac{1}{2}}x^{\gamma_++1}}\,\mathrm{d}x \lesssim 1 + \lambda^{\frac{1+p\alpha}{2(\gamma_++1)}} \int_0^\infty y^{p\alpha} e^{-pcy^{\gamma_++1}}\,\mathrm{d}y. \tag{22.88}$$

The case $p = \infty$ can be checked by calculating the maximum of $|f|$ and the second case for $x \lesssim -1$ is analogous. □

The immediate consequence is a possibility to employ pseudomodes constructed for V even for $V + W$, where W is an L^r-perturbation.

Theorem 22.2. *Let Assumption 22.1 hold and set $n := N - 1$. Let $\Im V$ satisfy* (22.82) *and* (22.84) *and let $W \in L^{r_-}(\mathbb{R}_-) + L^{r_+}(\mathbb{R}_+)$ with some $2 \leq r_\pm < \infty$. Then*

$$\frac{\|(H_{V+W} - \lambda)f\|}{\|f\|} = \kappa(\lambda) + \sigma^{(n)}(\lambda) + \rho(\lambda), \tag{22.89}$$

where f, κ and $\sigma^{(n)}$ are as in Theorem 22.1 and $\rho = \rho_- + \rho_+$ with

$$\rho_\pm(\lambda) = \mathcal{O}\left(\lambda^{\frac{\gamma-\gamma_\pm-\frac{2}{r_\pm}(\gamma+1)}{4(\gamma_\pm+1)(\gamma+1)}}\right), \qquad \lambda \to +\infty, \tag{22.90}$$

where γ and $\gamma_\pm$ are as in Lemma 22.5.

Proof. The estimate follows from (22.83), (22.85) with $\alpha = 0$ and Hölder inequality. In detail, with $2/r_\pm + 2/s_\pm = 1$, we have

$$\frac{\|Wf\|_{L^2(\mathbb{R}_\pm)}}{\|f\|} \leq \frac{\|W\|_{L^{r_\pm}(\mathbb{R}_\pm)}\|f\|_{L^{s_\pm}(\mathbb{R}_\pm)}}{\|f\|} \lesssim \lambda^{\frac{2(\gamma+1)-s_\pm(\gamma_\pm+1)}{4s_\pm(\gamma+1)(\gamma_\pm+1}} \tag{22.91}$$

and the claim follows when $s_\pm$ is expressed in terms of $r_\pm$. □

The weighted L^p-estimates of f can be used also to employ the pseudomode with $n = N$, instead of $n = N - 1$ in Theorem 22.1, and thereby lower assumptions on the regularity of V.

Theorem 22.3. *Let Assumption 22.1 hold and set $n := N$. Let $\Im V$ satisfy* (22.82) *and* (22.84) *and let $V^{(N+1)} \in L^2(\mathbb{R}) + L^\infty_{-\alpha_-}(\mathbb{R}_-) + L^\infty_{-\alpha_+}(\mathbb{R}_+)$ with some $\alpha_\pm \geq 0$. Then*

$$\frac{\|(H_V - \lambda)f\|}{\|f\|} = \kappa(\lambda) + \sigma^{(n)}(\lambda) + \tau(\lambda), \tag{22.92}$$

where f is the pseudomode with $n = N$, κ and $\sigma^{(n)}$ are as in Theorem 22.1 and $\tau = \tau_- + \tau_+$ with

$$\tau_\pm(\lambda) = \mathcal{O}\left(\lambda^{-\frac{N+1}{2}-\frac{1}{4(\gamma+1)}} + \lambda^{-\frac{N+1}{2}+\frac{\gamma-\gamma_\pm+2\alpha_\pm(\gamma+1)}{4(\gamma_\pm+1)(\gamma+1)}}\right), \qquad \lambda \to +\infty, \tag{22.93}$$

where γ and $\gamma_\pm$ are as in Lemma 22.5.

Proof. If f is taken as the pseudomode with $n = N$, the terms κ and $\sigma^{(n)}$ in (22.92) are estimated in the same way as in Theorem 22.1. The difference arises in the first term of r_n, see (22.25), since it contains $V^{(N+1)}$, more precisely, we need to estimate

$$\lambda^{-\frac{N+1}{2}}\|V^{(N+1)}f\|. \tag{22.94}$$

The claim follows straightforwardly from assumption on $V^{(N+1)}$, Hölder inequality, (22.83) and (22.85). □

22.4.2 Examples

Example 22.4 (Singularly perturbed polynomial-like potentials)**.** Let V be as in Example 22.1 and $W \in L^{r_-}(\mathbb{R}_-) + L^{r_+}(\mathbb{R}_+)$ with $2 \le r_\pm < \infty$. If Assumption 22.1 holds with $N \ge 2$, Theorem 22.2 and the already obtained rates $\sigma^{(n)}$, see Example 22.1 and in particular (22.73), yield

$$\begin{aligned}\frac{\|(H_{V+W}-\lambda)f\|}{\|f\|} &= \mathcal{O}\left(\lambda^{-\frac{1}{2r_\pm(\gamma+1)}}\right) + \begin{cases}\mathcal{O}\left(\lambda^{-\frac{N}{2}}\right), & \omega \le N,\\ \mathcal{O}\left(\lambda^{-\frac{N}{2}+\frac{\omega-N}{2(\gamma+1)+\epsilon(\omega-N)}}\right) & \omega > N,\end{cases}\\ &= \mathcal{O}\left(\lambda^{-\frac{1}{2r_\pm(\gamma+1)}}\right),\end{aligned} \tag{22.95}$$

as $\lambda \to +\infty$. Here the second equality follows by the restrictions made on β and γ in Example 22.1 (*cf* particularly (22.73)). In other words, adding the singularity W deteriorates the decay rate (22.72) (at least by using the result of Theorem 22.2).

Example 22.5 (Imaginary step-like potential)**.** Now we would like to treat the discontinuous example from (22.5). First, to apply Theorem 22.2, we specify a suitable splitting (to have a sufficiently regular V)

$$V(x) := i(1-\eta(x))\operatorname{sgn}(x), \qquad W(x) := i\eta(x)\operatorname{sgn}(x), \tag{22.96}$$

with some $\eta \in C_0^\infty((-1,1))$ and $\eta = 1$ on a neighbourhood of 0. Then Theorem 22.2 (with $N \ge 1$, $r_\pm := 2$ and $\gamma_\pm := 0 =: \gamma$) yields

$$\frac{\|(H_{i\,\mathrm{sgn}}-\lambda)f\|}{\|f\|} = \mathcal{O}\left(\lambda^{-\frac{1}{4}}\right), \qquad \lambda \to +\infty. \tag{22.97}$$

Example 22.6 (Polynomial growth with a local singularity)**.** As an application of Theorem 22.3, let us consider the following class of potentials

$$V(x) := i\ \operatorname{sgn}(x)\,|x|^\gamma\left(2+\sin|x|^{-\mu}\right), \qquad \mu \in (0,1)\,,\ \gamma \in \mathbb{N}\,.$$

If $\gamma \ge 2$ and $N := \gamma - 1$, it is easy to verify that V satisfies also the other items of Assumption 22.1 (with $\nu_\pm := -1$), namely the basic regularity requirement $V \in W^{N,\infty}(\mathbb{R})$. Since the derivative $V^{(\gamma)}$ has a singularity at zero, however, the best decay rate we can obtain by directly applying Theorem 22.1 is

$$\frac{\|(H_V-\lambda)f\|}{\|f\|} = \mathcal{O}\left(\lambda^{-\frac{\gamma-1}{2}+\frac{1}{2(\gamma+1)}+\epsilon}\right), \qquad \lambda \to +\infty, \tag{22.98}$$

where $\epsilon > 0$ can be made arbitrarily small (*cf* (22.71)). On the other hand, observing that $V^{(\gamma)} \in L^2(\mathbb{R})+L^\infty(\mathbb{R})$ and applying Theorem 22.3 (with $\alpha_\pm := 0$ and $\gamma_\pm := \gamma$), where a pseudomode with one more term in the expansion is employed, we obtain a better result, namely

$$\frac{\|(H_V-\lambda)f\|}{\|f\|} = \mathcal{O}\left(\lambda^{-\frac{\gamma}{2}}\right), \qquad \lambda \to +\infty. \tag{22.99}$$

22.4.3 Mollification strategy

Now we turn to the alternative approach to deal with irregular potentials.

Let $w \in C_0^\infty(\mathbb{R})$ with $0 \le w \le 1$, $\operatorname{supp} w = [-1,1]$ and $\|w\|_1 = 1$ and define

$$w_\varepsilon(x) := \frac{1}{\varepsilon}\,w\left(\frac{x}{\varepsilon}\right), \qquad x \in \mathbb{R}, \quad \varepsilon > 0. \tag{22.100}$$

For $\phi \in L^p_{\mathrm{loc}}(\mathbb{R})$, we introduce the L^p modulus of continuity on an interval $\mathcal{J} \subset \mathbb{R}$ by

$$\omega_p(\varepsilon;\phi,\mathcal{J}) := \sup_{0<|t|<\varepsilon}\|\phi(\cdot+t)-\phi\|_{L^p(\mathcal{J})}, \qquad 1 \le p < \infty. \tag{22.101}$$

Finally, we introduce an ε-neighbourhood of $\mathcal{J}$, $\mathcal{J}_\varepsilon := \{x \in \mathbb{R} : \operatorname{dist}(x,\mathcal{J}) < \varepsilon\}$.

The main idea in what follows is the mollification of a singular part of the potential. For $\phi \in L^p_{\mathrm{loc}}(\mathbb{R})$ and w_ε as in (22.100), we denote

$$\phi^\varepsilon := w_\varepsilon * \phi. \tag{22.102}$$

To be able to estimate newly constructed pseudomodes, we need several basic properties of mollifications and their relation to the L^p modulus of continuity summarised in the following lemma; the proof relies on Minkowski's integral inequality and properties of the convolution and of w.

Lemma 22.6. *Let $\phi \in L^p_{\mathrm{loc}}(\mathbb{R})$ with $1 \le p < \infty$, ϕ^ε be as in* (22.102)*, $\mathcal{J}$ be an interval and $\mathcal{J}_\varepsilon$ its ε-neighbourhood. Then for every $1 \le p < \infty$, $j \in \mathbb{N}$ and $\varepsilon > 0$ we have*

$$\|\phi^\varepsilon\|_{L^p(\mathcal{J})} \le \|\phi\|_{L^p(\mathcal{J}_\varepsilon)}, \qquad \|\phi^\varepsilon\|_{L^\infty(\mathcal{J})} \le \varepsilon^{-\frac{1}{p}} \|\phi\|_{L^p(\mathcal{J}_\varepsilon)}, \tag{22.103}$$

$$\|\phi - \phi^\varepsilon\|_{L^p(\mathcal{J})} \le \omega_p(\varepsilon; \phi, \mathcal{J}), \qquad \|(\phi^\varepsilon)^{(j)}\|_{L^p(\mathcal{J})} \le \varepsilon^{-j}\, \omega_p(\varepsilon; \phi, \mathcal{J})\, \|w^{(j)}\|_{L^1}. \tag{22.104}$$

We proceed with the construction of pseudomodes for a potential $V+W$ where W is possibly discontinuous and singular. In fact the pseudomodes are constructed for $V + W^\varepsilon$ with certain λ-dependent mollification. Thus besides usual remainders (22.22) we need to estimate also $\|(W - W^\varepsilon)f\|$.

While construction can be in principle performed with an arbitrary number of terms, we restrict ourselves to the case $n \in [[0,1]]$ since assumptions on the singular part W would become more complicated and implicit for $n > 1$. In spite of this restriction, we can still treat potentials with $\nu_\pm < 0$, *i.e.* even with some super-polynomial growth or oscillations. More precisely, new pseudomodes are constructed under the following assumptions.

Assumption 22.2. Let V satisfy Assumption 22.1 with $N \in [[1,2]]$ and $\nu_\pm < 0$ and suppose that $W = W_1 + W_2$ satisfy

a) $|\Im W_1| \le (1-\varepsilon)|\Im V|$ with some $0 < \varepsilon < 1$ and with $\varepsilon_1 > 0$ from Assumption 22.1

$$\forall x \in \mathbb{R}_\pm, \quad |\Re W_1(x)| \lesssim |\Im V(x)|^2 \langle x\rangle^{-4(\nu_\pm + \varepsilon_1) - 2}. \tag{22.105}$$

b) $W_2 \in L^2(\mathbb{R})$ and $\operatorname{supp} W_2$ is compact.

The mollification (22.102) is done separately for three parts of W, namely

$$\tilde{W} := (\chi_- W_1)^{\varepsilon_-} + (\chi_+ W_1)^{\varepsilon_+} + W_2^{\varepsilon_0} \tag{22.106}$$

with $\chi_\pm$ being the characteristic function of $\mathbb{R}_\pm$ and

$$\varepsilon_\iota := \lambda^{-\alpha_\iota}, \quad \alpha_\iota \in (0,1), \quad \iota \in \{-,+,0\}. \tag{22.107}$$

The expansion (see (22.11))

$$\tilde{g} := \exp\left(-\sum_{k=-1}^{n-1} \lambda^{-\frac{k}{2}} \psi_k(x)\right), \quad n \le 1, \tag{22.108}$$

is determined by functions ψ_k' satisfying (22.26) with V replaced by

$$\tilde{V} := V + \tilde{W}. \tag{22.109}$$

On the other hand, we keep the size of the cut-off the same as for V only, *i.e.* the new pseudomodes read

$$\tilde{f} := \xi \tilde{g}, \tag{22.110}$$

where ξ is as in (22.12) with $\delta_\pm$, $\Delta_\pm$ as in (22.35) with V.

Lemma 22.7. *Let Assumption 22.2 hold and $\tilde{g}$ be as in* (22.108) *with* (22.109)*. Then*

$$\kappa(\lambda) := \frac{\|\xi''\tilde{g}\| + \|\xi'\tilde{g}'\|}{\|\tilde{g}\|} = o(1), \quad \lambda \to +\infty, \tag{22.111}$$

with κ as in (22.58) *(with possibly a smaller positive constant $c > 0$).*

Proof. We start with showing

$$\|\tilde{f}\|^2 \gtrsim \int_{\mathcal{J}} \exp\left(-c_3 \lambda^{-\frac{1}{2}} \int_0^{|x|} |\Im V(t)|\, \mathrm{d}t\right) \mathrm{d}x \tag{22.112}$$

with some $c_3 > 0$, where $\tilde{f}$ is defined in (22.110). We give details on estimates on $\mathbb{R}_+$, the other case is analogous. First notice that $\tilde{W}$ is locally bounded, see Lemma 22.6. Moreover, since $\varepsilon_\pm = o(\Delta_\pm)$, we obtain from (22.29), (22.33) and assumptions on W that

$$\begin{aligned}
|\Im(\chi_\pm W_1)^{\varepsilon_\pm}(x)| &\le \int_{\mathbb{R}} w_{\varepsilon_\pm}(y) |\Im W_1(x-y)|\, \mathrm{d}y \le \sup_{|y|<\varepsilon_\pm} |\Im W_1(x-y)| \\
&\le (1-\varepsilon) \sup_{|y|<\varepsilon_\pm} |\Im V(x-y)| \\
&\le (1-\varepsilon)\left(|\Im V(x)| + \sup_{|y|<\varepsilon_\pm}\left|\int_x^{x-y} |\Im V'(t)|\, \mathrm{d}t\right|\right), \\
&\le (1-\varepsilon)|\Im V(x)|(1 + \mathcal{O}(\varepsilon_\pm))
\end{aligned} \tag{22.113}$$

and similarly, using (22.105) and (22.33),

$$\forall x \in \mathbb{R}_\pm, \quad |\Re(\chi_\pm W_1)^{\varepsilon_\pm}(x)| \lesssim |\Im V(x)|^2 \langle x\rangle^{-4(\nu_\pm+\varepsilon_1)-2}. \tag{22.114}$$

For W_2, Lemma 22.6 yields immediately

$$|W_2^{\varepsilon_0}(x)| \le \varepsilon_0^{-\frac{1}{2}} \|W_2\| = o\left(\lambda^{\frac{1}{2}}\right), \quad \lambda \to +\infty. \tag{22.115}$$

The estimates above imply that $\tilde{W}$ can actually be absorbed by V or λ in all relevant estimates in Lemmata 22.3, 22.4 and Proposition 22.1; in particular notice that W_2 affects the estimates only on a compact set due to the assumed boundedness of $\operatorname{supp} W_2$, and that the size of $\Re\tilde{W}$ is the largest possible complying with (22.30) and (22.35). Straightforward estimates of (22.50) with $n \in [[0,1]]$ and with V replaced by $\tilde{V}$ lead to (with some $c_1, c_2 > 0$)

$$e^{-c_1\lambda^{-\frac{1}{2}}\int_0^{|x|}|\Im V(t)|\,\mathrm{d}t} \lesssim |\tilde{g}(x)| \lesssim e^{-c_2\lambda^{-\frac{1}{2}}\int_0^{|x|}|\Im V(t)|\,\mathrm{d}t} \tag{22.116}$$

for $n \in [[0,1]]$, all sufficiently large λ and all $x \in \mathcal{J}$; here (22.113), (22.114), (22.115) and the boundedness of $\operatorname{supp} W_2$ were used. Hence (22.112) follows.

To verify (22.111), we need in addition that

$$\forall x \in \mathcal{J}_\pm, \quad |((\chi_+ W_1)^{\varepsilon_\pm})'(x)| \lesssim \frac{|\Im V(x)| + |\Im V(x)|^2\langle x\rangle^{-4(\nu_\pm+\varepsilon_1)-2}}{\varepsilon_\pm}; \tag{22.117}$$

the proof si similar to (22.113) and (22.114). Hence, using (22.26), (22.117) and (22.107), we obtain

$$\forall x \in \mathcal{J}_\pm, \quad \lambda^{\frac{1}{2}}|\psi_{-1}'(x)| + |\psi_0'(x)| \lesssim \lambda^{\frac{1}{2}} + |V(x)| + |\Im V(x)|^2\langle x\rangle^{-4(\nu_\pm+\varepsilon_1)-2}. \tag{22.118}$$

The rest of the proof is a simple modification of the one of Proposition 22.1. ☐

Now we are in a position to state the main result of this section.

Theorem 22.4. *Let Assumption 22.2 hold and $\tilde{f}$ be as in* (22.110) *with $n \in [[0,1]]$. Then*

$$\frac{\|(H_{V+W}-\lambda)\tilde{f}\|}{\|\tilde{f}\|} = \kappa(\lambda) + \sigma^{(n)}(\lambda) + \frac{\zeta^{(n)}(\lambda)}{\|\tilde{f}\|}, \tag{22.119}$$

where κ and $\sigma^{(n)}$ are as in Theorem 22.1 and $\zeta^{(n)} = \zeta_-^{(n)} + \zeta_+^{(n)} + \zeta_0^{(n)}$ with, as $\lambda \to +\infty$,

$$\begin{aligned}
\zeta_\pm^{(0)}(\lambda) &= \mathcal{O}\Big(\omega_2(\varepsilon_\pm; W_1, \mathcal{J}_\pm)\left(1+\varepsilon_\pm^{-1}\lambda^{-\frac{1}{2}}\right)\Big),\\
\zeta_0^{(0)}(\lambda) &= \mathcal{O}\Big(\omega_2(\varepsilon_0; W_2, \mathbb{R})\left(1+\varepsilon_0^{-1}\lambda^{-\frac{1}{2}}\right)\Big),\\
\zeta_\pm^{(1)}(\lambda) &= \mathcal{O}\Big(\omega_2(\varepsilon_\pm; W_1, \mathcal{J}_\pm)\left(1+\varepsilon_\pm^{-2}\lambda^{-1}\right) + \omega_4(\varepsilon_\pm; W_1, \mathcal{J}_\pm)\varepsilon_\pm^{-2}\lambda^{-2}\Big),\\
\zeta_0^{(1)}(\lambda) &= \mathcal{O}\Big(\omega_2(\varepsilon_0; W_2, \mathbb{R})\left(1+\varepsilon_0^{-2}\lambda^{-1}\right) + \omega_4(\varepsilon_0; W_2, \mathbb{R})\varepsilon_0^{-2}\lambda^{-2}\Big),
\end{aligned} \tag{22.120}$$

where ε_ι are as in (22.107).

Proof. Inserting the pseudomode $\tilde{f}$, we obtain

$$\|(H_{V+W}-\lambda)\tilde{f}\| \le \|(H_{\tilde{V}}-\lambda)\tilde{f}\| + \|(\tilde{W}-W)\tilde{f}\|. \tag{22.121}$$

We need to estimate remainders (22.22) with $\tilde{V}$ and the second term in (22.121). The claim follows straightforwardly from (22.27) and the properties of mollification, see Lemma 22.6. ☐

22.4.4 Examples

First we prove a lemma on L^p modulus of continuity of a piece-wise C^1 potentials with a controlled growth.

Lemma 22.8. *Let W be a piece-wise C^1 function, more precisely $W \in C^1(\mathbb{R} \setminus \mathcal{M})$ with $\mathcal{M} := \{a_k\}_{k\in\mathbb{Z}}$ such that for all $k \in \mathbb{Z}$, $a_{k+1} - a_k \gtrsim 1$ and for all $k \in \mathbb{Z}$ the one-sided limits $\lim_{x\to a_{k\pm}} W(x)$ exist and are finite. Moreover, let W satisfy*

$$\exists \beta_\pm \in \mathbb{R}, \quad \forall x \in \mathbb{R}_\pm, \quad |W(x)| \lesssim \langle x\rangle^{\beta_\pm}, \tag{22.122}$$

and

$$\exists \gamma_\pm \in \mathbb{R}, \quad \forall x \in \mathbb{R}_\pm \setminus \mathcal{M}, \quad |W'(x)| \lesssim \langle x \rangle^{\gamma_\pm}. \tag{22.123}$$

Then, for all ε *small and* $\delta_\pm$ *large,*

$$\omega_p(\varepsilon; W, \mathcal{J}_\pm) \lesssim \varepsilon \delta_\pm^{\gamma_\pm + \frac{1}{p}} + \varepsilon^{\frac{1}{p}} \delta_\pm^{\beta_\pm + \frac{1}{p}}, \quad 2 \leq p < \infty. \tag{22.124}$$

If in addition $\operatorname{supp} W$ *is bounded, then*

$$\omega_p(\varepsilon; W, \mathbb{R}) \lesssim \varepsilon^{\frac{1}{p}}, \quad 2 \leq p < \infty. \tag{22.125}$$

Proof. We analyse only the case with $\mathcal{J}_+$, the other situation being analogous. We can assume that $a_0 = 0$ and $a_{L+1} = \delta_+$ with some $L \in \mathbb{N}$. Splitting the intervals (a_k, a_{k+1}) to ε-neighbourhoods of the discontinuities and the rest and employing the assumptions on W and W', we have, for every $|t| < \varepsilon$,

$$\begin{aligned}
\int_{\mathcal{J}_+} |W(x+t) - W(x)|^p \, \mathrm{d}x &= \sum_{k=0}^{L} \int_{a_k}^{a_{k+1}} |W(x+t) - W(x)|^p \, \mathrm{d}x \\
&= \sum_{k=0}^{L} \int_{a_k}^{a_{k+1}-\varepsilon} \left| \int_x^{x+t} W'(\xi) \, \mathrm{d}\xi \right|^p \mathrm{d}x + \sum_{k=0}^{L} \int_{a_{k+1}-\varepsilon}^{a_{k+1}} |W(x+t) - W(x)|^p \, \mathrm{d}x \\
&\lesssim \sum_{k=0}^{L} \int_{a_k}^{a_{k+1}-\varepsilon} \mathrm{d}x \left(\operatorname*{ess\,sup}_{(a_0-\varepsilon, a_{L+1})} |W'| \right)^p \varepsilon^p + \sum_{k=0}^{L} \int_{a_{k+1}-\varepsilon}^{a_{k+1}} \mathrm{d}x \sup_{(a_{k+1}-\varepsilon, a_{k+1}+\varepsilon)} |W|^p \\
&\lesssim \delta_+^{1+p\gamma_+} \varepsilon^p + \varepsilon \sum_{k=0}^{L} a_{k+1}^{p\beta_+}.
\end{aligned}$$

Consequently, (22.124) follows since $a_{k+1} - a_k \gtrsim 1$ and the last sum can be estimated by an integral (details are omitted).

If $\operatorname{supp} W$ is bounded, then the estimates are performed on a bounded interval independent of $\delta_\pm$ and so (22.125) follows as well. ☐

Example 22.7 (Imaginary step-like potential continued)**.** Following Example 22.5, we keep the splitting of the imaginary sign potential $i\,\mathrm{sgn}$ to the sum of the smooth potential V and the discontinuous W of compact support, see (22.96). The latter obeys Assumption 22.2 with $W_1 := 0$. Applying Theorem 22.4 (with $n := 1$ and $\alpha_0 := 1/2$ in (22.107)) with help of Lemma 22.5 (with $\gamma := 0$ and $p := 2$) to estimate $\|\tilde{f}\|$ and Lemma 22.8 to estimate the moduli of continuity in $\zeta^{(1)}(\lambda)$, we arrive at

$$\frac{\|(H_{i\,\mathrm{sgn}} - \lambda)\tilde{f}\|}{\|\tilde{f}\|} = \mathcal{O}\left(\lambda^{-\frac{1}{2}}\right), \qquad \lambda \to +\infty\,.$$

This is an improvement with respect to the rate $\lambda^{-\frac{1}{4}}$ provided by Theorem 22.2, see Example 22.5. Nevertheless, even this better rate is not optimal, as it is known from [9] that there exists a pseudomode with the decay rate $O(\lambda^{-1})$ and that it is actually the best possible.

Example 22.8 (Infinite steps)**.** Let us consider the step-like (odd) potential

$$U(x) := i \, \lfloor |x| \rfloor^\gamma \, \mathrm{sgn}(x)\,, \qquad \gamma > 0\,, \tag{22.126}$$

where $\lfloor \cdot \rfloor$ denotes the floor function. Hence U represents a piece-wise approximation of $x \mapsto i\,|x|^\gamma \,\mathrm{sgn}(x)$ (*cf* Example 22.1 with $P_\beta := 0$). The basic hypothesis (22.28) is clearly satisfied, so it is expected that H_U admits pseudomodes. However, Theorem 22.1 cannot be used because of the lack of regularity required by Assumption 22.1.

We show how Theorem 22.4 can be used instead. To this end, we split U as

$$U = V + W\,, \qquad W = W_1 + W_2\,, \tag{22.127}$$

where

$$\begin{aligned}
V(x) &:= i\,(1 - \eta(x))\,|x|^\gamma \,\mathrm{sgn}(x)\,, \\
W_1(x) &:= i\,(1 - \eta(x))\,(\lfloor |x| \rfloor^\gamma - |x|^\gamma)\,\mathrm{sgn}(x)\,, \\
W_2(x) &:= i\eta(x)\,\lfloor |x| \rfloor^\gamma \,\mathrm{sgn}(x)\,,
\end{aligned} \tag{22.128}$$

and $\eta \in C_0^\infty(\mathbb{R})$ is such that $0 \le |\eta| \le 1$ and $\eta = 1$ on the interval $[-\gamma-1, \gamma+1]$. Using the mean value theorem and properties of the floor function, we have

$$|W_1(x)| \le (1-\eta(x))\,\gamma\,|x|^{\gamma-1}\,\big|\lfloor |x| \rfloor - |x|\big| \le (1-\eta(x))\,\gamma\,|x|^{\gamma-1} \tag{22.129}$$

for every $x \in \mathbb{R}$. Since $W_1(x)$ equals zero if $|x| \le \gamma+1$, we see that Assumption 22.2 clearly holds with $\varepsilon := 1/(\gamma+1)$.

Now we are in a position to apply Theorem 22.4 with $n := 1$. For $\sigma^{(1)}(\lambda)$, we always have a decay, see Example 22.1. Lemma 22.5 with $p := 2$ yields

$$\|\tilde{f}\| \gtrsim \lambda^{\frac{1}{4(\gamma+1)}} \tag{22.130}$$

for all sufficiently large λ and Lemma 22.8 immediately implies (we take $\alpha_0 := 1/2$)

$$\zeta_0^{(1)}(\lambda) = \mathcal{O}\left(\lambda^{-\frac{1}{4}}\right), \qquad \lambda \to +\infty\,. \tag{22.131}$$

Again from Lemma 22.8 (with $\beta_\pm := \gamma - 1$ and $\gamma_\pm$ arbitrarily large negative), we obtain for W_1 (with $\alpha_\pm := \alpha \in (0,1)$)

$$\lambda^{-\frac{1}{4(\gamma+1)}}\,\omega_p(\lambda^{-\alpha}; W_1, \mathcal{J}_\pm) = \mathcal{O}\left(\lambda^{-\frac{\alpha}{p}+\frac{1}{2p(\gamma+1)}+\frac{2\gamma-3}{4(\gamma+1)}+\epsilon}\right), \qquad \lambda \to +\infty, \tag{22.132}$$

where $\epsilon = \epsilon(\gamma,p) > 0$ can be made arbitrarily small. Calculating the individual terms in $\zeta_\pm^{(1)}$, we obtain the following conditions on α to have a decay in (22.119):

$$\frac{\gamma-1}{\gamma+1} < \alpha < \frac{1}{3}\frac{\gamma+3}{\gamma+1}\,. \tag{22.133}$$

These can be satisfied only if $\gamma < 3$ and the corresponding decay rate in (22.119) can be calculated in a straightforward way.

22.5 Pseudomodes for general curves

In this section, we focus on potentials V with unbounded $\Im V$ and investigate pseudomodes for other curves in the complex plane than lines parallel to the real axis. The construction is basically the same as in Section 22.3, however, instead of having the pseudomode localised around 0, we work around a λ-dependent point.

As the support of the pseudomode will be contained in $\mathbb{R}_+$, this construction is suitable also for operators in $L^2(\mathbb{R}_+)$. In fact we shall rather proceed reversely and formulate the strategy for such a situation, the subsequent applicability of the results for problems in $L^2(\mathbb{R})$ being obvious.

22.5.1 Admissible class of potentials and curves

To keep the previous strategy working without more complicated and implicit conditions on V, we add an additional condition on $\Im V$, namely a control of $\Im V'(x)$. In detail, we assume the following.

Assumption 22.3. Let $N \in \mathbb{N}$, $N > 1$, let $V \in W^{N,\infty}_{\mathrm{loc}}(\overline{\mathbb{R}_+})$ satisfy

$$\lim_{x\to+\infty} \Im V(x) = +\infty \tag{22.134}$$

together with all the conditions of Assumption 22.1 for $x > 0$. In addition suppose that

$$\forall x \gtrsim 1, \qquad \Im V'(x) \gtrsim \Im V(x)\langle x\rangle^{\nu}, \tag{22.135}$$

where $\nu := \nu_+$.

In this section, we write

$$\lambda = a + ib, \qquad a \in \mathbb{R},\ b \in \mathbb{R}_+. \tag{22.136}$$

For sufficiently large b we define the *turning point* x_b of $\Im V$ by the equation

$$\Im V(x_b) = b, \tag{22.137}$$

which is well-defined due to (22.135). The cut-off is taken around the turning point x_b, namely:

$$\begin{aligned} &\xi \in C_0^\infty(\mathbb{R}_+), \quad 0 \le \xi \le 1, \\ &\forall x \in (x_b - \delta + \Delta, x_b + \delta - \Delta), \quad \xi(x) = 1, \\ &\forall x \notin (x_b - \delta, x_b + \delta), \quad \xi(x) = 0. \end{aligned} \tag{22.138}$$

Here we take

$$\delta := \frac{x_b^{-\nu}}{2}, \qquad \Delta := \frac{\delta}{4}, \tag{22.139}$$

and denote

$$\mathcal{J}_b := (x_b - \delta, x_b + \delta), \qquad \mathcal{J}_b' := (x_b - \delta + \Delta, x_b + \delta - \Delta). \tag{22.140}$$

Finally, we restrict the real part of λ by

$$\forall x \in \mathcal{J}_b, \qquad b^{\frac{2}{3}} x_b^{\frac{2\nu}{3}} \lesssim |a| \lesssim a - \Re V(x) \lesssim b^2 x_b^{-4\nu - 4\varepsilon_1 - 2}. \tag{22.141}$$

The set of admissible a's is non-empty since $\sup_{x \in \mathcal{J}_b} |\Re V(x)| \lesssim b^2 x_b^{-4\nu-4\varepsilon_1-2}$ by assumption (22.30) and the choice of $\mathcal{J}_b$ in (22.140); moreover it follows from (22.30) that $b^{\frac{2}{3}} x_b^{\frac{2\nu}{3}} \lesssim b^2 x_b^{-4\nu-4\varepsilon_1-2}$ for every sufficiently small $\varepsilon_1 > 0$.

22.5.2 Pseudomode construction

The pseudomode will have the form

$$f(x) := \xi(x) g(x) \qquad \text{with} \qquad g(x) := \exp\left(- \sum_{k=-1}^{n-1} \lambda^{-\frac{k}{2}} \int_{x_b}^{x} \psi_k'(t) \, \mathrm{d}t \right), \tag{22.142}$$

where $\{\psi_k'\}_{k \in [[-1, n-1]]}$ are determined by (22.21).

Proposition 22.2. *Let Assumption 22.3 hold,* $0 \le n \le N$, $\{\psi_k'\}_{k \in [[-1,n-1]]}$ *be determined by* (22.21), $\mathcal{J}_b$, $\mathcal{J}_b'$ *be as in* (22.140), ξ, g *be as in* (22.138), (22.142), *respectively, and* a *satisfy* (22.141). *Then there exists* $c > 0$ *such that*

$$\frac{\|\xi'' g\|_{L^2(\mathbb{R}_+)} + \|\xi' g'\|_{L^2(\mathbb{R}_+)}}{\|\xi g\|_{L^2(\mathbb{R}_+)}} = \mathcal{O}(\exp(-c x_b^{\nu+1+2\varepsilon_1})), \quad b \to +\infty. \tag{22.143}$$

Proof. Let us first estimate $\operatorname{sgn}(x - x_b) \int_{x_b}^{x} \Re(\lambda^{\frac{1}{2}} \psi_{-1}'(t)) \, \mathrm{d}t$. For $x_b < x < x_b + \delta$ (the other case is analogous), an analogue of the the complex square root formula (22.31), the choice of a in (22.141) and the mean value theorem lead to

$$\begin{aligned} \Re(\lambda^{\frac{1}{2}} \psi_{-1}'(x)) &\gtrsim \frac{\Im V(x) - b}{(a - \Re V(x))^{\frac{1}{2}} + (\Im V(x) - b)^{\frac{1}{2}}} \\ &\gtrsim \frac{\Im V'(x_b)(x - x_b)}{|a|^{\frac{1}{2}} + (\Im V'(x_b)(x - x_b))^{\frac{1}{2}}}. \end{aligned} \tag{22.144}$$

In the second inequality we have also used that the values of $\Im V'$ at $\mathcal{J}_b$ are comparable, see (22.29) and (22.33). Hence, for every $x \in \mathcal{J}_b \setminus \mathcal{J}_b'$, we have

$$\int_{x_b}^{x} \Re(\lambda^{\frac{1}{2}} \psi_{-1}'(t)) \, \mathrm{d}t \gtrsim \frac{b \, x_b^{-\nu}}{|a|^{\frac{1}{2}} + b^{\frac{1}{2}}} \gtrsim \begin{cases} x_b^{\nu+1+2\varepsilon_1}, & |a| > b, \\ b^{\frac{1}{2}} \, x_b^{-\nu}, & |a| \le b. \end{cases} \tag{22.145}$$

Here the first inequality employs (22.135) in the numerator and (22.29) in the denominator, while the second inequality follows from (22.141). Notice that by (22.30) we have $b^{\frac{1}{2}} \, x_b^{-\nu} \gtrsim x_b^{\nu+1+2\varepsilon_1}$, so the left hand side tends to infinity as $b \to +\infty$ too.

Next we investigate $\int_{x_b}^{x} |\lambda^{-\frac{k}{2}} \psi_k'|$ for $k \in [[0, n-1]]$ and $x \in \mathcal{J}_b$. The estimates analogous to (22.46), (22.47) and the choice of a in (22.141) yield

$$\int_{x_b}^{x} |\lambda^{-\frac{k}{2}} \psi_k'(t)| \, \mathrm{d}t \lesssim \sum_{j=1}^{k+1} \int_{x_b}^{x} \frac{|V(t)|^j x_b^{(k+1)\nu}}{|a - \Re V(t)|^{j+\frac{k}{2}}} \, \mathrm{d}t \lesssim \sum_{j=1}^{k+1} \frac{(|a|^j + b^j) x_b^{k\nu}}{|a|^{j+\frac{k}{2}}}. \tag{22.146}$$

Further from (22.141) and (22.30)

$$\sum_{j=1}^{k+1} \frac{|a|^j x_b^{k\nu}}{|a|^{j+\frac{k}{2}}} \lesssim \left(\frac{x_b^{\nu}}{|a|^{\frac{1}{2}}} \right)^k \lesssim \left(\frac{x_b^{2\nu}}{b} \right)^{\frac{k}{3}} \lesssim x_b^{-\frac{2}{3}k(\nu+1+\varepsilon_1)} \tag{22.147}$$

and

$$\sum_{j=1}^{k+1} \frac{b^j x_b^{k\nu}}{|a|^{j+\frac{k}{2}}} \lesssim \begin{cases} x_b^{-k(\nu+1+\varepsilon_1)}, & |a| > b, \\ \sum_{j=1}^{k+1} \left(b x_b^{-2\nu} \right)^{\frac{j-k}{3}}, & |a| \le b. \end{cases} \tag{22.148}$$

Thus, using again (22.30), for every $x \in \mathcal{J}_b \setminus \mathcal{J}_b'$ we get

$$\frac{\int_{x_b}^x |\lambda^{-\frac{k}{2}}\psi_k'(t)|\,\mathrm{d}t}{\int_{x_b}^x \Re(\lambda^{\frac{1}{2}}\psi_{-1}'(t))\,\mathrm{d}t} \lesssim x_b^{-(\frac{2}{3}k+1)(\nu+1+\varepsilon_1)} + \begin{cases} x_b^{-(k+1)(\nu+1+\varepsilon_1)}, & |a| > b, \\ x_b^{-(\nu+1+\varepsilon_1)}, & |a| \le b. \end{cases} \tag{22.149}$$

Using (22.145) with help of (22.149) and (22.13), we obtain (with some $C_1 > 0$)

$$\|\xi'' g\|_{L^2(\mathbb{R}_+)} + \|\xi' g'\|_{L^2(\mathbb{R}_+)} \lesssim \exp\left(-C_1 \frac{b x_b^{-\nu}}{|a|^{\frac{1}{2}} + b^{\frac{1}{2}}}\right). \tag{22.150}$$

The estimate is clear for the first norm on the left hand side. To control the extra terms obtained by differentiating g, we employ the bounds coming from Gronwall's inequality (22.32) for the term $\lambda^{\frac{1}{2}}\psi_{-1}'$ and the other terms $\lambda^{-\frac{k}{2}}\psi_k'$ can be estimated similarly as in (22.146).

Finally, to show (22.143), we need to verify that $\|\xi g\|_{L^2(\mathbb{R}_+)}$ is not too small. To this end notice that for $a < b$

$$\begin{aligned} \int_{x_b}^{x_b + x_b^{-2|\nu|}} |\Re(\lambda^{\frac{1}{2}}\psi_{-1}'(t))|\,\mathrm{d}t &\lesssim \int_{x_b}^{x_b + x_b^{-2|\nu|}} |\Im V(t) - b|^{\frac{1}{2}}\,\mathrm{d}t \\ &\lesssim b^{\frac{1}{2}} x_b^{-3|\nu| + \frac{1}{2}\nu} \end{aligned} \tag{22.151}$$

and for $a \ge b$

$$\begin{aligned} \int_{x_b}^{x_b + x_b^{-2|\nu|}} |\Re(\lambda^{\frac{1}{2}}\psi_{-1}'(t))|\,\mathrm{d}t &\lesssim \int_{x_b}^{x_b + x_b^{-2|\nu|}} \frac{\Im V'(x_b)(t - x_b)}{|a|^{\frac{1}{2}}}\,\mathrm{d}t \\ &\lesssim |a|^{-\frac{1}{2}} b\, x_b^{\nu - 4|\nu|}. \end{aligned} \tag{22.152}$$

Since

$$\begin{cases} b^{\frac{1}{2}} x_b^{-3|\nu| + \frac{1}{2}\nu} = o\left(\dfrac{b\, x_b^{-\nu}}{|a|^{\frac{1}{2}} + b^{\frac{1}{2}}}\right), & a < b, \\ |a|^{-\frac{1}{2}} b\, x_b^{\nu - 4|\nu|} = o\left(\dfrac{b\, x_b^{-\nu}}{|a|^{\frac{1}{2}} + b^{\frac{1}{2}}}\right), & a \ge b, \end{cases} \tag{22.153}$$

we obtain in both cases (with some $C_2 > 0$)

$$\frac{\|\xi'' g\|_{L^2(\mathbb{R}_+)} + \|\xi' g'\|_{L^2(\mathbb{R}_+)}}{\|\xi g\|_{L^2(\mathbb{R}_+)}} \lesssim \exp\left(-C_2 \frac{b\, x_b^{-\nu}}{|a|^{\frac{1}{2}} + b^{\frac{1}{2}}}\right). \tag{22.154}$$

The claim (22.143) follows from the last inequality in (22.145). ☐

Theorem 22.5. *Let Assumption 22.3 hold, f be as in* (22.142) *with $n = N - 1$ and a satisfy* (22.141). *Then, as $b \to +\infty$,*

$$\begin{aligned} \frac{\|(H_V - \lambda) f\|_{L^2(\mathbb{R}_+)}}{\|f\|_{L^2(\mathbb{R}_+)}} = \mathcal{O}\Bigg(&\exp(-c x_b^{\nu+1+2\varepsilon_1}) + x_b^{N\nu} \sup_{x \in \mathcal{J}_b} \frac{b + |\Re V(x)|}{(a - \Re V(x))^{\frac{N}{2}}} \\ &+ \sum_{k=0}^{N-2} \sum_{l=2}^{N+k} x_b^{(N+k)\nu} \sup_{x \in \mathcal{J}_b} \frac{(b + |\Re V(x)|)^l}{(a - \Re V(x))^{\frac{N-2+k}{2} + l}}\Bigg). \end{aligned} \tag{22.155}$$

Proof. The claim follows straightforwardly from Proposition 22.2, the estimate of the remainder $|r_n|$, see (22.25), and the choice of a, see (22.141). ☐

Example 22.9 (Example 22.1 continued)**.** We illustrate applicability of Theorem 22.5 on the imaginary monomial potentials, namely $V(x) = ix^\gamma$ for $x > 0$ and $\gamma \ge 1$. With this choice, we have $\nu = -1$, $x_b = b^{\frac{1}{\gamma}}$ and we may take a as (with $\varepsilon > 0$)

$$b^{\frac{2}{3}\frac{\gamma-1}{\gamma} + \varepsilon} \lesssim a \lesssim b^{2\frac{\gamma+1}{\gamma} - \varepsilon}, \tag{22.156}$$

see (22.141). Straightforward calculations yield that for a sufficiently large N we get a decay in (22.155). In other words we show that there are pseudomodes (with a decay in (22.155)) in the region bounded by curves $\Gamma_{1,2}$ in $\mathbb{C}$ given by

$$\Gamma_1(t) := t^{\frac{2}{3}\frac{\gamma-1}{\gamma} + \varepsilon} + it, \qquad \Gamma_2(t) := t^{2\frac{\gamma+1}{\gamma} - \varepsilon} + it. \tag{22.157}$$

Notice that for $\gamma = 2$, we obtain (with obvious re-parametrisation) curves $\eta + i\eta^p$ with $1/3 < p < 3$ of the Boulton's conjecture, *cf* [4], which are known to be optimal, *cf* [18].

Example 22.10 (Semiclassical operators)**.** Let us briefly explain how the semiclassical setting, see *e.g.* [5], can be treated using our approach and how previously used assumptions can be relaxed. For a sufficiently regular potential U, we search for pseudomodes of the semiclassical operator

$$-h^2\frac{\mathrm{d}^2}{\mathrm{d}x^2}+U(x)-z, \quad h>0, \tag{22.158}$$

corresponding to a pseudoeigenvalue $z\in\mathbb{C}$, in the limit $h\to 0$.

First we factor the parameter h^2 out and obtain (22.1) with the scaled potential $V(x):=h^{-2}U(x)$ and pseudoeigenvalue $\lambda:=h^{-2}z$ in our notations, see (22.2). The pseudomode is constructed around the point x_0 satisfying the equation $\Im V(x_0)=\Im\lambda$, *i.e.* $\Im U(x_0)=\Im z$. Notice that x_0 is determined only by $\Im z$, which is fixed here.

The cut-off is successful if there are $\delta_\pm$ such that for all $x\in(x_0+\delta_+/2, x_0+\delta_+)$

$$\int_{x_0}^{x}\frac{\Im U(t)-\Im U(x_0)}{(\Re z-\Re U(t))^{\frac12}+|\Im U(t)-\Im U(x_0)|^{\frac12}}\,\mathrm{d}t\gtrsim h^{1-\varepsilon} \tag{22.159}$$

with some $\varepsilon>0$ and similarly for δ_-. Indeed, appropriately modified first inequality in (22.144) yields

$$\Re(\lambda^{\frac12}\psi'_{-1}(t))\gtrsim h^{-1}\frac{\Im U(t)-\Im U(x_0)}{(\Re z-\Re W(t))^{\frac12}+|\Im U(t)-\Im U(x_0)|^{\frac12}}. \tag{22.160}$$

However, (22.159) can be satisfied *e.g.* when Davies' condition [5]

$$\Im U'(x_0)>0 \qquad \text{and} \qquad z=\eta^2+U(x_0) \quad \text{with} \quad \eta^2>0 \tag{22.161}$$

is imposed; indeed, Taylor's theorem yields

$$\begin{aligned}\Im U(t)-\Im U(x_0)&=\Im U'(x_0)(t-x_0)+\mathcal{O}((t-x_0)^2),\\ \Re z-\Re U(t)&=\eta^2+\mathcal{O}(|t-x_0|), \qquad\qquad t\to x_0,\end{aligned} \tag{22.162}$$

and so the choice $\delta_+:=h^{\frac{1-\varepsilon}{2}}$ works. It can be also easily checked that the other terms in the expansion are harmless. Finally, the decay of the remainders r_n follows easily if $|\Re z-\Re U(x)|$ is not too small on $(x_0-\delta_-, x_0+\delta_+)$, which is satisfied when Davies' condition (22.161) holds; as an illustration, we have

$$h^2|r_0|\lesssim\frac{h}{|\Re z-\Re U(x)|^{\frac12}} \tag{22.163}$$

for all $x\in(x_0-\delta_-, x_0+\delta_+)$.

In summary, the semiclassical setting allows for many simplifications and a suitable behaviour of U around a fixed point x_0 only is needed to obtain pseudomodes (localising around x_0) as $h\to 0$. It is also clear that the previously used conditions of the type $\Im U'(x_0)\neq 0$ are not needed as we may use larger neighbourhood of x_0 and take sufficiently large η to satisfy (22.159) and obtain a decay of r_n.

Example 22.11 (Strong local singularities)**.** In all previous pseudomode constructions, we used the behaviour of the potential V at infinity. If V is sufficiently singular at a finite point, the construction of the present Section 22.5 can be adapted accordingly. We illustrate this on an example in $L^2(\mathbb{R}_-)$ with

$$V(x):=\frac{i}{|x|^\alpha} \qquad \text{for} \qquad x\in(-1,0), \qquad \alpha>2, \tag{22.164}$$

and arbitrary behaviour outside $(-1,0)$. We consider $\mathbb{R}_-$ for convenience only so that (22.134) holds for $x\to 0-$ and the shape of already derived formulas is preserved. Considering $\mathbb{R}_+$ instead of $\mathbb{R}_-$ and further generalisations in the sense of Section 22.5.1 (like $\Re V\neq 0$ or $\nu>-1$) are straightforward. We emphasise in particular the potentials with $\Re V(x)=c/|x|^2$, $c\in\mathbb{R}$, appearing in the radial part of higher-dimensional Schrödinger operators.

We follow the notations of Section 22.5.1 and construct a pseudomode of the type (22.142) around the turning point x_b of $\Im V$ that tends to $0-$ as $b\to+\infty$. In more detail, we take here

$$\begin{aligned}\lambda&=a+ib, \qquad a,b\in\mathbb{R}_+,\\ \Im V(x_b)&=b, \qquad \delta:=\frac{|x_b|}{2}, \quad \Delta:=\frac{\delta}{4},\end{aligned} \tag{22.165}$$

with δ going to zero as $b \to \infty$, and the cut-off ξ as well as intervals $\mathcal{J}_b$ and $\mathcal{J}'_b$ are as in (22.138), (22.140), respectively. The new condition on admissible a's (corresponding to the simple case (22.164)) reads

$$b^{\frac{2}{3}(1+\frac{1}{\alpha})} \lesssim a \lesssim b^{2(1-\frac{1}{\alpha})-\epsilon} \tag{22.166}$$

with some $\epsilon > 0$.

Following and slightly adapting the estimates in the proof of Proposition 22.2, we get for every $x \in \mathcal{J}_b \setminus \mathcal{J}'_b$ with $x > x_b$ that

$$\int_{x_b}^{x} \Re(\lambda^{\frac{1}{2}} \psi'_{-1}(t))\, \mathrm{d}t \gtrsim \frac{b^{1-\frac{1}{\alpha}}}{a^{\frac{1}{2}} + b^{\frac{1}{2}}}. \tag{22.167}$$

Here the importance of the assumed condition $\alpha > 2$, as well as (22.166), is clearly visible in order to ensure that the right-hand side tends to infinity as $b \to +\infty$. It can be further checked straightforwardly that the cut-off is indeed successful and an analogue of (22.154) holds; we remark that in estimates like (22.151) and (22.152) we integrate *e.g.* over $(x_b, x_b + x_b^2)$.

The remainder estimate is also straightforward, using (22.25), we obtain altogether that with V as in (22.164) there is a positive constant c such that

$$\frac{\|(H_V - \lambda)f\|_{L^2(\mathbb{R}_-)}}{\|f\|_{L^2(\mathbb{R}_-)}} = \mathcal{O}\left(\exp(-cb^{\frac{\epsilon}{2}}) + \frac{b^{1+\frac{n+1}{\alpha}}}{a^{\frac{n+1}{2}}} + \sum_{k=0}^{n-1} \sum_{l=2}^{n+1+k} \frac{b^{l+\frac{n+1+k}{\alpha}}}{a^{l+\frac{n-1+k}{2}}} \right) \tag{22.168}$$

as $b \to +\infty$ (then necessarily also $a \to +\infty$ due to (22.166)). Similarly as in Example 22.9, we can check that if we strengthen (22.166) to

$$b^{\frac{2}{3}(1+\frac{1}{\alpha})+\epsilon} \lesssim a \lesssim b^{2(1-\frac{1}{\alpha})-\epsilon} \tag{22.169}$$

with some $\epsilon > 0$, then for a sufficiently large n we indeed have a decay in (22.168).

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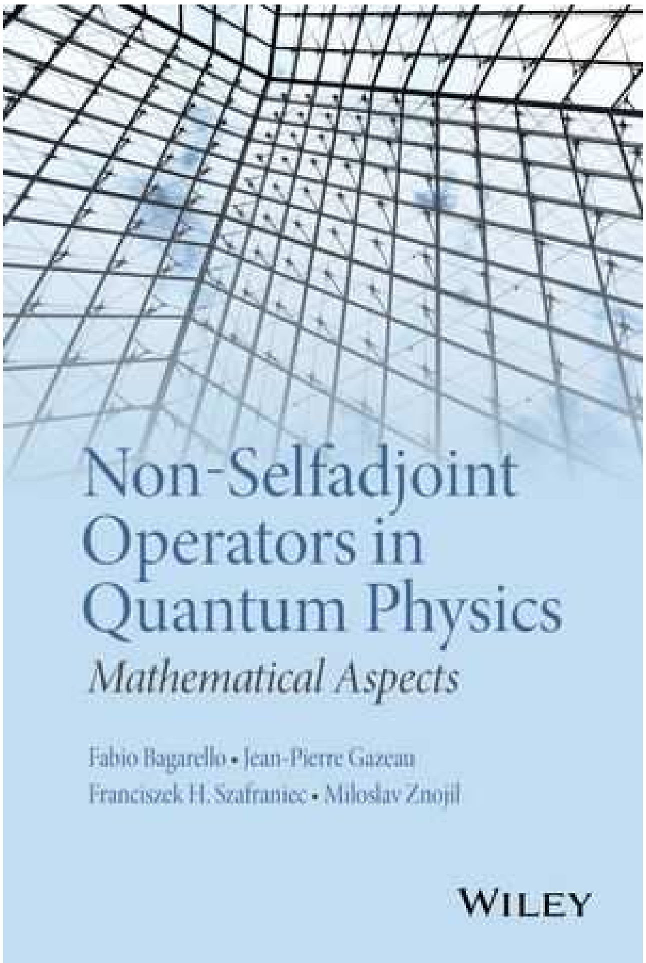
Appendix

Appendix A

Elements of Spectral Theory without the Spectral Theorem



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Joint work with: Petr Siegl

Elements of spectral theory without the spectral theorem

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A.1 Introduction

Many physical systems can be described by partial differential equations and the latter can often be viewed as generating abstract operators between Banach spaces. A typical example is quantum mechanics where the traditional mathematical discipline is the functional analysis of self-adjoint operators in Hilbert spaces. There are also effective models (typically describing open quantum systems, including non-real fields or complex boundary conditions) or more generally non-conservative processes in Nature on the whole where the underlying operator is non-self-adjoint. More intrinsically, there have been recent attempts to build quantum mechanics with physical observables represented by non-self-adjoint operators.

From the mathematical point of view, the theory of self-adjoint operators is well understood, while the non-self-adjoint theory is still in its infancy. Or maybe more appropriate would be to say that the theory is "underdeveloped", as spectral theory of non-self-adjoint operators is an equally old branch of functional analysis. Indeed, the first pioneering works (1908–1913) of G. D. Birkhoff on non-self-adjoint boundary value problems were written almost at the same time as D. Hilbert's famous papers (1904–1910) that initiated self-adjoint spectral theory (*cf* [61, p. viii]). But it was not until M. V. Keldyš' work (1951) when first abstract results on non-self-adjoint problems appeared in the literature, while the self-adjoint theory was already enjoying all the pleasures of life due to the needs of quantum mechanics at that time.

It is frustrating that the powerful techniques of the self-adjoint theory, such as the spectral theorem and variational principles, are not available for non-self-adjoint operators. Moreover, recent studies have revealed that this lack of tools is fundamental; the non-self-adjointness may lead to new and unexpected phenomena. Although there exist many interesting observations coming from physics and numerical studies of non-self-adjoint operators, the deep theoretical understanding is still missing. The problem is that the non-self-adjoint theory is much more diverse and it is difficult, if not impossible, to find a common thread. *Indeed it can hardly be called a theory.* This is a quotation from the preface of E. B. Davies' 2007 book [17], where a significant amount of work on spectral theory of non-self-adjoint operators can be found. The author continues:

Studying non-self-adjoint 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.

We fully endorse this opinion and understand that the only way how "to acquire the much wider range of knowledge" is by studying many distinct cases. This chapter is particularly concerned with various cases coming from the rapidly developing field of quantum mechanics with non-self-adjoint operators. But we hope the present material will be useful for anybody interested in methods of spectral theory when the spectral theorem is not available.

The structure of this chapter is as follows. The forthcoming Section A.2 is mainly devoted to a collection of basic facts from the spectral theory of operators in Hilbert spaces. In Section A.3 we summarise some efficient methods how to construct a closed operator with non-empty resolvent set. The theory of compact operators and various definitions of essential spectra are recalled in Section A.4. Section A.5 is concerned with operators which are similar to self-adjoint (or more generally normal) operators. Finally, in Section A.6, we recall the notion of pseudospectra as a more reliable information about non-self-adjoint operators than the spectrum itself.

Our exposition is in many respects based on the classical monographs [23, 34] to which we refer for statements presented here without (or just sketchy) proofs. In addition to these references, we also use the new edition [1] about Sobolev spaces, which are denoted here by $H^m(\Omega)$, and the book [29] about partial differential equations. Other references are quoted in the text. The majority of the material is standard, but we illustrate the abstract exposition by some unconventional quantum-mechanically motivated examples.

A.2 Closed operators in Hilbert spaces

Having in mind the applications of differential operators in quantum mechanics, we concentrate on closed operators acting in *Hilbert spaces*, although many concepts summarised below are relevant in Banach spaces as well.

A.2.1 Basic notions

Throughout this chapter $\mathcal{H}$ stands for a separable Hilbert space over the complex number field $\mathbb{C}$. The norm and inner product (antilinear in the first component) in $\mathcal{H}$ will be denoted by $\|\cdot\|$ and $(\cdot,\cdot)$, respectively. A paradigmatic example is the Lebesgue space $L^2(\Omega)$ of square-integrable functions over an open set $\Omega \subset \mathbb{R}^d$.

We define a *linear operator* H in $\mathcal{H}$ to be a pair consisting of a linear subspace $\mathsf{D}(H) \subset \mathcal{H}$ called the *domain* of H and a linear map $H : \mathsf{D}(H) \to \mathcal{H}$. If $\mathsf{D}(H)$ is dense in $\mathcal{H}$, H is said to be *densely defined*. The image $\mathsf{R}(H) := H\mathsf{D}(H)$ is called the *range* of H. The *null space* or *kernel* $\mathsf{N}(H)$ of H is the set of all $\psi \in \mathsf{D}(H)$ such that $H\psi = 0$.

If H_1 and H_2 are two operators in $\mathcal{H}$ such that $\mathsf{D}(H_1) \subset \mathsf{D}(H_2)$ and $H_1\psi = H_2\psi$ for all $\psi \in \mathsf{D}(H_1)$, we write $H_1 \subset H_2$ and say that H_2 is an *extension* of H_1 and H_1 is a *restriction* of H_2.

The following quantities play an important role in spectral theory:

$$
\begin{aligned}
&\textit{nullity}, && \mathsf{nul}(H) := \dim \mathsf{N}(H)\,, \\
&\textit{deficiency}, && \mathsf{def}(H) := \operatorname{codim} \mathsf{R}(H)\,.
\end{aligned}
$$

Recall that the codimension of a subspace $\mathcal{H}' \subset \mathcal{H}$ is defined as the dimension of the quotient space $\mathcal{H}/\mathcal{H}'$. If $\mathcal{H}'$ is closed, then $\operatorname{codim}\mathcal{H}' = \dim \mathcal{H}'^{\perp}$, where $\perp$ denotes the orthogonal complement, but this equality does not extend to non-closed subspaces, as the following example shows.

Example A.1 (Identity operator)**.** The *identity operator* I in $L^2(\mathbb{R})$, *i.e.* $I\psi := \psi$, $\mathsf{D}(I) := L^2(\mathbb{R})$, has a closed range, $\mathsf{R}(I) = L^2(\mathbb{R})$, by definition, so $\mathsf{def}(I) = 0$. The situation is very different for its restriction $I'\psi := I\psi$, $\mathsf{D}(I') := C_0^\infty(\mathbb{R})$, when $\mathsf{R}(I') = C_0^\infty(\mathbb{R})$. Since $\mathsf{R}(I')$ is dense in $L^2(\mathbb{R})$, we have $\dim \mathsf{R}(I')^\perp = 0$. However, $\mathsf{R}(I')$ is not closed and $\mathsf{def}(I') = +\infty$; indeed, for instance Hermite functions are supported everywhere in $\mathbb{R}$ and form an orthonormal basis of $L^2(\mathbb{R})$.

The operator $H : \mathsf{D}(H) \to \mathcal{H}$, understood as a mapping between two normed spaces $(\mathsf{D}(H), \|\cdot\|)$ and $\mathcal{H}$, is said to be *bounded* if there exists a non-negative number M such that $\|H\psi\| \le M\|\psi\|$ for all $\psi \in \mathsf{D}(H)$. The smallest number M with this property is called the *norm* of H and is denoted by $\|H\|_{\mathsf{D}(H)\to\mathcal{H}}$, *i.e.*

$$
\|H\|_{\mathsf{D}(H)\to\mathcal{H}} := \sup_{\psi\in\mathsf{D}(H),\psi\neq 0,} \frac{\|H\psi\|}{\|\psi\|}.
$$

If H is bounded and $\mathsf{D}(H) = \mathcal{H}$, *i.e.* H is an operator *on* $\mathcal{H}$ to $\mathcal{H}$, we drop the subscript in the notation of the norm, *i.e.* $\|H\| := \|H\|_{\mathcal{H}\to\mathcal{H}}$. The space of all bounded operators on $\mathcal{H}$ to $\mathcal{H}$ is denoted by $\mathscr{B}(\mathcal{H})$. H is bounded if and only if it is *continuous*, *i.e.*,

$$
\mathsf{D}(H) \ni \psi_n \xrightarrow[n\to\infty]{} \psi \in \mathsf{D}(H) \quad \Longrightarrow \quad H(\psi_n - \psi) \xrightarrow[n\to\infty]{} 0\,.
$$

Most of the physically relevant operators are unbounded, including differential operators in $L^2(\Omega)$.

A suitable substitute for the continuity in the more general situation of unbounded operators is the important notion of closedness. We say that H is *closed* if

$$
\left.
\begin{aligned}
\mathsf{D}(H) \ni \psi_n \xrightarrow[n\to\infty]{} \psi \in \mathcal{H} \\
H\psi_n \xrightarrow[n\to\infty]{} \phi \in \mathcal{H}
\end{aligned}
\right\}
\quad \Longrightarrow \quad \big[\psi \in \mathsf{D}(H) \ \wedge \ H\psi = \phi\big]\,.
$$

Since the spectrum is defined *only* for closed operators, *cf* Section A.2.2, checking that a given operator H is closed should be the first step in any spectral analysis of H. In what follows, H is thus typically assumed to be a closed operator in $\mathcal{H}$.

We also assume that H is densely defined, which is convenient in order to have the unique *adjoint* H^* defined as follows

$$
\begin{aligned}
&\mathsf{D}(H^*) := \big\{\phi \in \mathcal{H} \,:\, \exists \phi^* \in \mathcal{H},\ \forall \psi \in \mathsf{D}(H),\ (\phi, H\psi) = (\phi^*, \psi)\big\}\,, \\
&H^*\phi := \phi^*\,.
\end{aligned}
\tag{A.1}
$$

H^* is always a closed operator, regardless whether H is closed or not, but it may happen that $\mathsf{D}(H^*) = \{0\}$. For any densely defined operator H, we have

$$
\mathsf{N}(H^*) = \mathsf{R}(H)^\perp\,. \tag{A.2}
$$

It turns out that differential operators in $L^2(\Omega)$ are closed and densely defined when their domains are properly chosen. We illustrate the situation on several characteristic examples coming from quantum mechanics.

Example A.2 (Multiplication operator)**.** Given an open set $\Omega \subset \mathbb{R}^d$, let M_V be the operator of *multiplication* in $L^2(\Omega)$ by a measurable function $V : \Omega \to \mathbb{C}$. It is defined by $M_V\psi := V\psi$ on its maximal domain $\mathsf{D}(M_V) := \{\psi \in L^2(\Omega) : V\psi \in L^2(\Omega)\}$. M_V is densely defined and closed. M_V is bounded on $L^2(\Omega)$ if and only if V is essentially bounded, in which case we have $\|M_V\| = \|V\|_\infty$. The adjoint of M_V is obtained by simply taking the complex conjugate of V, *i.e.* $M_V^* = M_{\overline{V}}$, in particular, $\mathsf{D}(M_V^*) = \mathsf{D}(M_V)$. A quantum-mechanically distinguished example is the *position operator* q in $L^2(\mathbb{R})$ which is associated with the choice $V(x) := x$.

Example A.3 (Momentum operator)**.** Given an open interval $\Omega \subset \mathbb{R}$, we introduce the *momentum* operator p in $L^2(\Omega)$ by $p\psi := -i\psi'$ and $\mathsf{D}(p) := H^1(\Omega)$. The operator p is densely defined, closed and always unbounded. The adjoint acts in the same way, but it satisfies an extra Dirichlet boundary condition on $\partial\Omega$, *i.e.* $p^*\psi = -i\psi'$ and $\mathsf{D}(p^*) = H_0^1(\Omega)$. In $L^2(\mathbb{R})$, p and q are unitarily equivalent via the Fourier transform.

Example A.4 (Creation and annihilation operators)**.** In $L^2(\mathbb{R})$, we introduce the *creation* and *annihilation* operators as follows. The annihilation operator is introduced as $a := ip + q$; by definition, $\mathsf{D}(a) = \mathsf{D}(p) \cap \mathsf{D}(q)$. The operator a is densely defined and it can be proved that it is closed and that its adjoint, the creation operator, reads $a^* = -ip + q$ (with $\mathsf{D}(a^*) = \mathsf{D}(a)$).

The famous harmonic-oscillator Hamiltonian

$$H_{\mathrm{HO}} := p^2 + q^2\,, \qquad \mathsf{D}(H_{\mathrm{HO}}) = \{\psi \in H^2(\mathbb{R}) \,:\, x^2\psi \in L^2(\mathbb{R})\}, \tag{A.3}$$

is closed and it can be verified that $H_{\mathrm{HO}} = a^*a + 1$, *i.e.* particularly the equality of the domains holds (notice that by definition of the product of two operators, $\mathsf{D}(a^*a) = \{\psi \in \mathsf{D}(a) \,:\, a\psi \in \mathsf{D}(a^*)\}$).

Example A.5 (Free Hamiltonian and constraints)**.** Given an open connected set Ω in $\mathbb{R}^d$, let us introduce an auxiliary densely defined operator $-\Delta^\Omega$ in $L^2(\Omega)$ which acts on the Sobolev space $\mathsf{D}(-\Delta^\Omega) := H^2(\Omega)$ as the Laplacian, *i.e.* $-\Delta^\Omega\psi := -\Delta\psi$. The case $\Omega = \mathbb{R}^d$ corresponds to the *free Hamiltonian* describing the motion a quantum particle in the whole space with the absence of external fields. It is well known that $-\Delta^{\mathbb{R}^d}$ is closed, in fact $-\Delta^{\mathbb{R}^d} = (-\Delta^{\mathbb{R}^d})^*$. If the boundary $\partial\Omega$ is not empty, a physically relevant closed realisation of $-\Delta^\Omega$ is typically obtained by imposing suitable boundary conditions. For sufficiently regular Ω, so that the boundary traces $H^2(\Omega) \hookrightarrow H^1(\partial\Omega)$ exist, we consider

$$\text{\textit{Dirichlet boundary conditions,}} \qquad \psi = 0 \quad \text{on} \quad \partial\Omega\,, \tag{A.4}$$

$$\text{\textit{Neumann boundary conditions,}} \qquad \frac{\partial\psi}{\partial n} = 0 \quad \text{on} \quad \partial\Omega\,, \tag{A.5}$$

$$\text{\textit{Robin boundary conditions,}} \qquad \frac{\partial\psi}{\partial n} + \alpha\,\psi = 0 \quad \text{on} \quad \partial\Omega\,, \tag{A.6}$$

where $\psi \in H^2(\Omega)$, n denotes the exterior unit normal vector field of $\partial\Omega$ and $\alpha : \partial\Omega \to \mathbb{C}$. We denote by $-\Delta_D^\Omega$, $-\Delta_N^\Omega$ and $-\Delta_\alpha^\Omega$ the operators in $L^2(\Omega)$ that act as $-\Delta^\Omega$ on smaller domains $\mathsf{D}(-\Delta_\iota^\Omega) := \{\psi \in H^2(\Omega) : (\iota) \text{ holds}\}$, where $\iota \in \{D, N, \alpha\}$ and (ι) stands for (A.4), (A.5) or (A.6), respectively. We call the operators the *Dirichlet*, *Neumann* and *Robin Laplacians*, respectively. All these operators are closed if Ω and α are sufficiently regular (*e.g.* Ω bounded with boundary of class C^2 and $\alpha \in C^1(\partial\Omega)$). Clearly, $-\Delta_N^\Omega = -\Delta_0^\Omega$, while $-\Delta_D^\Omega$ can be formally considered as corresponding to the extreme situation "$\alpha = \infty$".

A.2.2 Spectra

An *eigenvalue* of H is defined as a complex number λ such that the equation $H\psi = \lambda\psi$ has a non-zero solution $\psi \in \mathsf{D}(H)$ called *eigenvector*. In other words, λ is an eigenvalue of H if the null space $\mathsf{N}(H - \lambda)$ is not $\{0\}$; this null space is the *geometric eigenspace* for λ and the nullity $\mathsf{m}_{\mathrm{g}}(\lambda) := \mathsf{nul}(H - \lambda)$ is called the *geometric multiplicity* of λ. The *algebraic* (or *root*) *eigenspace* for λ is defined by

$$\mathsf{M}_\lambda := \bigcup_{n=1}^{\infty} \mathsf{N}([H - \lambda]^n)\,,$$

non-zero elements of M_λ are called *generalised eigenvectors* (or *root vectors*) corresponding to λ and $\mathsf{m}_{\mathrm{a}}(\lambda) := \dim \mathsf{M}_\lambda$ is called the *algebraic multiplicity* of λ. Obviously, $\mathsf{m}_{\mathrm{a}}(\lambda) \geq \mathsf{m}_{\mathrm{g}}(\lambda)$, where the inequality can be strict in general.

Example A.6 (Matrices with degenerate eigenvalues)**.** The nilpotent matrix $H := \left(\begin{smallmatrix} 0 & 1 \\ 0 & 0 \end{smallmatrix}\right)$ on $\mathbb{C}^2$ has only one eigenvalue $\lambda = 0$ with an eigenvector $\left(\begin{smallmatrix} 1 \\ 0 \end{smallmatrix}\right)$ and a generalised eigenvector $\left(\begin{smallmatrix} 0 \\ 1 \end{smallmatrix}\right)$, so $\mathsf{m}_{\mathrm{g}}(0) = 1$ and $\mathsf{m}_{\mathrm{a}}(0) = 2$. On the other hand, the null matrix $H := \left(\begin{smallmatrix} 0 & 0 \\ 0 & 0 \end{smallmatrix}\right)$ has one eigenvalue $\lambda = 0$ with two eigenvectors $\left(\begin{smallmatrix} 1 \\ 0 \end{smallmatrix}\right)$ and $\left(\begin{smallmatrix} 0 \\ 1 \end{smallmatrix}\right)$, so $\mathsf{m}_{\mathrm{g}}(0) = 2 = \mathsf{m}_{\mathrm{a}}(0)$. The null (infinite) matrix on $l^2(\mathbb{N})$ has $\lambda = 0$ as an eigenvalue of infinite geometric and algebraic multiplicities (as in fact has the null operator on any infinite-dimensional Hilbert space) and it is straightforward to construct examples of matrices with arbitrary values of $\mathsf{m}_{\mathrm{g}}(\lambda)$ and $\mathsf{m}_{\mathrm{a}}(\lambda)$.

More interesting examples of (differential) operators will be presented later.

The set of all eigenvalues of H is called

the *point spectrum*, $$\sigma_{\mathrm{p}}(H) := \{\lambda \in \mathbb{C} : \mathsf{N}(H-\lambda) \neq \{0\}\}.$$

If $\lambda \notin \sigma_{\mathrm{p}}(H)$, then the inverse $(H-\lambda)^{-1}$ exists. The *resolvent set* $\rho(H)$ of H is defined to be the set of all λ's for which $(H-\lambda)^{-1} \in \mathscr{B}(\mathcal{H})$, *i.e.* the inverse exists as a bounded operator on $\mathcal{H}$ (*i.e. on* $\mathcal{H}$ to $\mathcal{H}$). The operator-valued function $\lambda \mapsto (H-\lambda)^{-1}$ from $\rho(H)$ to $\mathscr{B}(\mathcal{H})$ is called the *resolvent* of H. The complement $\sigma(H) := \mathbb{C} \setminus \rho(H)$ is called the *spectrum* of H.

It is customary to introduce the spectrum for closed operators only, the reason being that the notion is trivial otherwise.

Proposition A.1. *If H is not closed, then $\sigma(H) = \mathbb{C}$.*

Proof. We prove it by contraposition: if $\lambda \in \rho(H) \neq \varnothing$, then $\mathsf{N}(H-\lambda) = \{0\}$ and $(H-\lambda)^{-1} \in \mathscr{B}(\mathcal{H})$. The latter implies that $(H-\lambda)^{-1}$ is closed. However, an invertible operator is closed if and only if its inverse is. Consequently, $H-\lambda$ and hence H are closed operators. □

In what follows we thus assume that H is a closed operator in $\mathcal{H}$.

The spectrum of operators in finite-dimensional Hilbert spaces is exhausted by eigenvalues. In general, however, there are additional subsets:

continuous spectrum, $$\sigma_{\mathrm{c}}(H) := \left\{\lambda \in \sigma(H) \setminus \sigma_{\mathrm{p}}(H) : \overline{\mathsf{R}(H-\lambda)} = \mathcal{H}\right\},$$

residual spectrum, $$\sigma_{\mathrm{r}}(H) := \left\{\lambda \in \sigma(H) \setminus \sigma_{\mathrm{p}}(H) : \overline{\mathsf{R}(H-\lambda)} \neq \mathcal{H}\right\}.$$

By the closed-graph theorem [34, Sec. III.5.4], the pathological situation of $\lambda \in \sigma(H)\setminus\sigma_{\mathrm{p}}(H)$ with $\mathsf{R}(H-\lambda) = \mathcal{H}$ cannot occur, therefore

$$\sigma(H) = \sigma_{\mathrm{p}}(H) \cup \sigma_{\mathrm{c}}(H) \cup \sigma_{\mathrm{r}}(H)$$

and the unions are disjoint. In other words, $\lambda \in \sigma(H)$ if and only if $H-\lambda$ is not bijective as an operator from $\mathsf{D}(H)$ to $\mathcal{H}$.

From the Neumann series for the resolvent, it follows that the resolvent set $\rho(H)$ is an open subset of $\mathbb{C}$, consequently the spectrum $\sigma(H)$ is closed (it can be empty or cover the whole complex plane).

The spectra of a densely defined closed operator H and its adjoint H^* are simply related via a mirror symmetry with respect to the real axis,

$$\forall \lambda \in \mathbb{C}, \qquad \lambda \in \sigma(H) \iff \overline{\lambda} \in \sigma(H^*).$$

However, the individual subsets of the spectrum may not satisfy this symmetry; in general, we have the following implications only.

Proposition A.2. *Let H be a densely defined closed operator and $\lambda \in \mathbb{C}$. Then*

$$\begin{aligned} &\bullet\ \lambda \in \sigma_{\mathrm{p}}(H) &&\Longrightarrow&& \overline{\lambda} \in \sigma_{\mathrm{p}}(H^*) \cup \sigma_{\mathrm{r}}(H^*), \\ &\bullet\ \lambda \in \sigma_{\mathrm{r}}(H) &&\Longrightarrow&& \overline{\lambda} \in \sigma_{\mathrm{p}}(H^*), \\ &\bullet\ \lambda \in \sigma_{\mathrm{c}}(H) &&\Longleftrightarrow&& \overline{\lambda} \in \sigma_{\mathrm{c}}(H^*). \end{aligned} \tag{A.7}$$

In particular,

$$\sigma_{\mathrm{r}}(H) = \left\{\lambda \in \mathbb{C} \setminus \sigma_{\mathrm{p}}(H) : \overline{\lambda} \in \sigma_{\mathrm{p}}(H^*)\right\}. \tag{A.8}$$

Proof. We prove the first two implications from which the rest follows. Let $\lambda \in \sigma_{\mathrm{p}}(H)$ and denote by ϕ the corresponding eigenvector. Then, for every $\psi \in \mathsf{D}(H^*)$, $((H^*-\overline{\lambda})\psi, \phi) = (\psi, (H-\lambda)\phi) = 0$, therefore $\mathsf{R}(H^*-\overline{\lambda})^{\perp} \neq \{0\}$, hence $\overline{\lambda} \notin \sigma_{\mathrm{c}}(H^*)$. Let $\lambda \in \sigma_{\mathrm{r}}(H)$, then (A.2) yields $\mathsf{N}(H^*-\overline{\lambda}) = \mathsf{R}(H-\lambda)^{\perp} \neq \{0\}$, hence $\overline{\lambda} \in \sigma_{\mathrm{p}}(H^*)$. □

Example A.7 (Spectrum of the multiplication operator)**.** In the full generality of Example A.2, we have

$$\begin{aligned} \sigma(M_V) &= \left\{\lambda \in \mathbb{C} : \left|\{x \in \Omega : \lambda - \varepsilon \leq V(x) \leq \lambda + \varepsilon\}\right| > 0 \text{ for all } \varepsilon\right\}, \\ \sigma_{\mathrm{p}}(M_V) &= \left\{\lambda \in \mathbb{C} : \left|\{x \in \Omega : V(x) = \lambda\}\right| > 0\right\}, \\ \sigma_{\mathrm{r}}(M_V) &= \varnothing, \end{aligned}$$

where $|\cdot|$ denotes the Lebesgue measure. Note that the spectrum of M_V equals the essential range of the function V. In particular, if V is continuous, then $\sigma(M_V)$ is the closure of the range of V. In the special case of the position operator q in $L^2(\mathbb{R})$, we have $\sigma(q) = \sigma_{\mathrm{c}}(q) = \mathbb{R}$.

Example A.8 (Spectrum of the momentum operator)**.** The spectrum of the momentum operator p from Example A.3 drastically depends on the choice of the configuration space Ω.

Ω	$\sigma_\mathrm{p}(p)$	$\sigma_\mathrm{c}(p)$	$\sigma_\mathrm{r}(p)$	$\sigma_\mathrm{p}(p^*)$	$\sigma_\mathrm{c}(p^*)$	$\sigma_\mathrm{r}(p^*)$
$\mathbb{R}$	$\varnothing$	$\mathbb{R}$	$\varnothing$	$\varnothing$	$\mathbb{R}$	$\varnothing$
$(0,+\infty)$	$\mathbb{C}^+$	$\mathbb{R}$	$\varnothing$	$\varnothing$	$\mathbb{R}$	$\mathbb{C}^-$
$(0,1)$	$\mathbb{C}$	$\varnothing$	$\varnothing$	$\varnothing$	$\varnothing$	$\mathbb{C}$

Here the notation $\mathbb{C}^\pm := \{\lambda \in \mathbb{C} : \Im\lambda \gtrless 0\}$ for the upper and lower half-plane is used.

Example A.9 (Spectrum of the creation and annihilation operators)**.** Recall Example A.4. We have $\sigma_\mathrm{c}(a) = \sigma_\mathrm{c}(a^*) = \varnothing$, $\sigma_\mathrm{p}(a) = \sigma_\mathrm{r}(a^*) = \mathbb{C}$ and $\sigma_\mathrm{r}(a) = \sigma_\mathrm{p}(a^*) = \varnothing$. The spectrum of the harmonic oscillator H_HO is given by algebraically simple eigenvalues $2n+1$ with $n = 0, 1, \dots$.

Example A.10 (Spectrum of the Laplacians)**.** The interesting dependence of the spectrum of the operators from Example A.5 on the geometry of Ω is out of the scope of the present chapter. We only mention the well-known result for the free Hamiltonian, $\sigma(-\Delta^{\mathbb{R}^d}) = \sigma_\mathrm{c}(-\Delta^{\mathbb{R}^d}) = [0,\infty)$, and henceforth focus on the one-dimensional situation $\Omega = (-a,a)$, $a > 0$. It is well known that

$$\sigma(-\Delta_N^{(-a,a)}) = \sigma_\mathrm{p}(-\Delta_N^{(-a,a)}) = \left\{\left(\frac{n\pi}{2a}\right)^2\right\}_{n=0}^{\infty},$$
$$\sigma(-\Delta_D^{(-a,a)}) = \sigma_\mathrm{p}(-\Delta_D^{(-a,a)}) = \left\{\left(\frac{n\pi}{2a}\right)^2\right\}_{n=1}^{\infty},$$

and all the eigenvalues are algebraically simple. The case of general Robin boundary conditions $\alpha : \partial\Omega \to \mathbb{C}$ is investigated in [40, 42]. In this one-dimensional situation it is natural to identify the function α with the couple $\{\alpha(-a), \alpha(+a)\}$. Here and in the sequel we consider only the special choice $\alpha(\pm a) = \pm i\alpha_0$ with $\alpha_0 \in \mathbb{R}$ that was originally introduced in [39, 38]. This choice admits an explicit solution

$$\sigma(-\Delta_{\{-i\alpha_0,i\alpha_0\}}^{(-a,a)}) = \sigma_\mathrm{p}(-\Delta_{\{-i\alpha_0,i\alpha_0\}}^{(-a,a)}) = \{\alpha_0^2\} \cup \left\{\left(\frac{n\pi}{2a}\right)^2\right\}_{n=1}^{\infty}.$$

Furthermore, it is easy to check that all the eigenvalues are algebraically simple provided that $2\alpha_0 a \notin \{\pm\pi, \pm 2\pi, \dots\}$, otherwise the eigenvalue α_0^2 is doubly degenerated with geometric and algebraic multiplicity one and two, respectively, and all the other eigenvalues are algebraically simple.

A.2.3 Numerical range

Despite of a usually direct physical interpretation of the spectrum, it is not an easily accessible quantity. Indeed, there is no hope to get such explicit formulae for the spectra as we did for the examples of the preceding section in the more general situation of differential operators with variable coefficients or defined on geometrically more complicated sets. The objective of the present subsection is to estimate the spectrum in terms of a more accessible quantity:

$$\textit{numerical range,} \qquad \Theta(H) := \{(\psi, H\psi) \,:\, \psi \in \mathsf{D}(H),\ \|\psi\| = 1\}.$$

In general, $\Theta(H)$ is neither open nor closed, even when H is a closed operator. It is, however, always convex. Let

$$\Xi(H) := \complement\overline{\Theta(H)} \equiv \mathbb{C} \setminus \overline{\Theta(H)} \tag{A.9}$$

denote the exterior of the numerical range of H. In view of the convexity of the numerical range, $\Xi(H)$ is either an open connected set or a union of two half-planes (for this reason we like to use the disconnected symbol Ξ to denote the exterior).

If $H \in \mathscr{B}(\mathcal{H})$, then the spectrum of H is a subset of the closure of $\Theta(H)$. More generally, we have

Proposition A.3. *Let H be a closed operator such that each connected component of $\Xi(H)$ has a non-empty intersection with $\rho(H)$. Then*

$$\sigma(H) \subset \overline{\Theta(H)} \qquad \textit{and} \qquad \|(H-\lambda)^{-1}\| \le \frac{1}{\operatorname{dist}\left(\lambda, \overline{\Theta(H)}\right)} \tag{A.10}$$

for every $\lambda \in \rho(H)$.

Proof. By Theorem [34, Sec. V.3.2], $\mathsf{R}(H-\lambda)$ is closed and $\mathsf{nul}(H-\lambda)=0$ for each $\lambda \in \Xi(H)$. Furthermore, $\lambda \mapsto \mathsf{def}(H-\lambda)$ is constant in each of the connected components of $\Xi(H)$. Consequently, if a connected component of $\Xi(H)$ has a non-empty intersection with $\rho(H)$, then it follows from (A.32) that this component is actually a subset of $\rho(H)$. This proves the set inclusion in the statement of the proposition. To show the inequality for the resolvent norm, we note that

$$\operatorname{dist}\left(\lambda, \overline{\Theta(H)}\right) \leq |(\psi, H\psi)-\lambda| = |(\psi,(H-\lambda)\psi)| \leq \|(H-\lambda)\psi\|$$

for any $\psi \in \mathsf{D}(H)$ with $\|\psi\|=1$ and every $\lambda \in \mathbb{C}$. Hence, the desired inequality follows by employing the fact that $\Xi(H)$ is a subset of $\rho(H)$ where $H-\lambda$ is bijective. ☐

Example A.11 (Numerical range of the momentum operator)**.** The assumption in Proposition A.3 about the intersection of the exterior of the numerical range with the resolvent set is absolutely necessary. We demonstrate it on the example of the momentum operator from Example A.3. The following table to be compared with that of Example A.8 shows that the spectrum cannot be controlled by the numerical range in general.

Ω	$\Theta(p)$	$\Theta(p^*)$
$\mathbb{R}$	$\mathbb{R}$	$\mathbb{R}$
$(0,+\infty)$	$\mathbb{C}$	$\mathbb{R}$
$(0,1)$	$\mathbb{C}$	$\mathbb{R}$

Indeed, we see that the spectrum is much larger than the numerical range of p^* on the half-line or bounded interval.

A.2.4 Sectoriality and accretivity

The extra condition in Proposition A.3 that ensures the useful properties (A.10) is of course annoying. The good news of this subsection is that there exists a distinguished class of operators for which we can do better. These are operators for which one can generically ensure that the exterior of the numerical range cannot have two connected components, by employing the convexity of the numerical range. We have already mentioned that it is the case of bounded operators, but this class of operators is insufficient for applications to differential operators. A fairly wide class is given by *sectorial* operators H defined by the property that their numerical range is a subset of a sector, *i.e.*,

$$\Theta(H) \subset S_{\gamma,\vartheta} := \{\lambda \in \mathbb{C} : \ |\arg(\lambda-\gamma)| \leq \vartheta\} \tag{A.11}$$

with some $\gamma \in \mathbb{R}$ and $0 \leq \vartheta < \pi/2$ called a *vertex* and a *semi-angle* of H, respectively. Since the inequality for the semi-angle is strict, the exterior $\Xi(H)$ is clearly a connected set.

It remains to state an extra property which would ensure that $\Xi(H)$ has a non-empty intersection with $\rho(H)$ provided that H is sectorial. This is done *ad hoc* by introducing the notion of m-sectoriality: H is said to be *m-sectorial* if it is sectorial and

$$\rho(H) \cap \complement\overline{S_{\gamma,\vartheta}} \neq \varnothing\,. \tag{A.12}$$

(The latter is equivalent to $\rho(H) \cap \Xi(H) \neq \varnothing$ due to the sectoriality.) Applying Proposition A.3, we may thus conclude with

Proposition A.4. *Let H be an m-sectorial operator. Then* (A.10) *holds.*

For applications, however, it is sometimes needed to allow the extreme situation $\vartheta = \pi/2$ in (A.11). H is said to be *quasi-accretive* if $\Theta(H) \subset S_{\gamma,\pi/2}$ with some $\gamma \in \mathbb{R}$ and it is said to be *accretive* if the vertex can be chosen at the origin, *i.e.* $\Theta(H) \subset S_{0,\pi/2}$. For the convenience of the reader, we summarise the various notions at one place here: an operator H is called

sectorial,	if (A.11) holds with	$\gamma \in \mathbb{R}$	and	$0 \leq \vartheta < \pi/2$,
accretive,	if (A.11) holds with	$\gamma = 0$	and	$0 \leq \vartheta \leq \pi/2$,
quasi-accretive,	if (A.11) holds with	$\gamma \in \mathbb{R}$	and	$0 \leq \vartheta \leq \pi/2$.

Again, we add the prefix m- to accretive if in addition (A.12) holds (which is now stronger than $\rho(H) \cap \Xi(H) \neq \varnothing$, since $\Xi(H)$ can have two disjoint components if $\vartheta = \pi/2$). Obviously, H is quasi-m-accretive if $H+\gamma$ is m-accretive with some $\gamma \in \mathbb{R}$ and H is m-sectorial if it is sectorial and quasi-m-accretive. Inspecting the proof of Proposition A.3, we easily check that H is m-accretive if and only if the standard requirements (*cf* [34, Eq. (V.3.38)])

$$\begin{aligned} &\bullet\quad \{\lambda \in \mathbb{C} : \ \Re\lambda < 0\} \subset \rho(H)\,, \\ &\bullet\quad \forall \lambda \in \mathbb{C},\ \Re\lambda < 0\,, \quad \|(H-\lambda)^{-1}\| \leq \frac{1}{|\Re\lambda|}\,, \end{aligned} \tag{A.13}$$

are satisfied.

The meaning of the m- terminology is that any m-accretive (respectively, m-sectorial) operator is *maximal* in the sense that it has no proper accretive (respectively, sectorial) extension (*cf* [34, Sec. V.3.10]). Furthermore, any m-accretive operator is automatically closed (*cf* Proposition A.1) and densely defined.

While checking the condition (A.11) on the numerical range for a given operator may be straightforward, more sophisticated tools are usually needed to verify (A.12). We shall be concerned with such methods in Section A.3.

The Laplacians from Example A.5 together with operators constructed from them by "small perturbations" (*cf* Section A.3.4) are m-sectorial. At the same time, the harmonic-oscillator Hamiltonian H_{HO} from Example A.4 is m-sectorial with vertex 1 and semi-angle 0. On the other hand, the momentum operators from Example A.3 (recall also Examples A.8 and A.11) are not even sectorial, although $\pm ip$ and $\pm ip^*$ on $\mathbb{R}$ as well as ip^* on the half-line are m-accretive. As a matter of fact, ip^* on the half-line is a warning example for the fact that no general variant of Proposition A.4 for quasi-m-accretive operators is available. Here we present other examples of quasi-accretive operators which are not sectorial:

Example A.12 (Imaginary Airy operator)**.** Consider in $L^2(\mathbb{R})$ the operator:

$$H_{\mathrm{Airy}} := p^2 + iq\,, \qquad \mathsf{D}(H_{\mathrm{Airy}}) = \{\psi \in H^2(\mathbb{R}) \,:\, x\psi \in L^2(\mathbb{R})\},$$

where p and q are introduced in Examples A.3 and A.2, respectively. H_{Airy} is m-accretive. The accretivity is simple to verify since, for all $\psi \in \mathsf{D}(H_{\mathrm{Airy}})$, the integration by parts yields $(\psi, H_{\mathrm{Airy}}\psi) = \|\psi'\|^2 + i(\psi, x\psi)$, whence $\Theta(H_{\mathrm{Airy}}) \subset S_{0,\pi/2}$. However, it is much more delicate to check (A.12) (*cf* Example A.24).

Example A.13 (Imaginary cubic oscillator)**.** The operator in $L^2(\mathbb{R})$:

$$H_{\mathrm{cubic}} := p^2 + iq^3\,, \qquad \mathsf{D}(H_{\mathrm{cubic}}) = \{\psi \in H^2(\mathbb{R}) \,:\, x^3\psi \in L^2(\mathbb{R})\},$$

is m-accretive. The reasoning is analogous to the previous example.

Example A.14 (Generator of the damped wave equation)**.** Given a bounded open connected set $\Omega \subset \mathbb{R}^d$ with smooth boundary $\partial\Omega$, consider the damped wave equation $u_{tt} + a(x)u_t - \Delta u = 0$, where $(x,t) \in \Omega \times (0,\infty)$ and $a \in L^\infty(\Omega)$ is real-valued, subject to Dirichlet boundary conditions $u(x,t) = 0$ for $(x,t) \in \partial\Omega \times (0,\infty)$ and initial conditions $u(\cdot,0) \in H^1(\Omega)$, $u_t(\cdot,0) \in L^2(\Omega)$. Writing $\psi := \binom{u}{u_t}$, the weak formulation of the differential equation leads to an abstract evolution problem $\psi_t = H_a\psi$ in the Hilbert space $\dot{H}^1_0(\Omega) \times L^2(\Omega)$ with $H_a := \begin{pmatrix} 0 & 1 \\ \Delta^\Omega_D & -a \end{pmatrix}$, $\mathsf{D}(H_a) := \mathsf{D}(-\Delta^\Omega_D) \times H^1_0(\Omega)$. Here $-\Delta^\Omega_D$ is the Dirichlet Laplacian from Example A.5 and $\dot{H}^1_0(\Omega)$ denotes the closure of $C^\infty_0(\Omega)$ with respect to the norm $\|\nabla \cdot\|$ (it is equivalent to the H^1_0-norm since we assume that Ω is bounded). H_a is m-accretive whenever $a \le 0$. We refer to [24, 25] for an application of spectral analysis of H_a to stability issues related to the damped wave equation.

As the last example suggests, quasi-accretive operators play an important role in evolution processes. In fact, by Hille-Yosida's theorem, *cf* [12, Thm. 7.4], a closed densely defined operator H in a Hilbert space $\mathcal{H}$ is a generator of a γ-contractive semigroup $T(t)$ (*i.e.* $\|T(t)\| \le e^{\gamma t}$ for all $t \ge 0$) if and only if $H + \gamma$ is m-accretive.

A.2.5 Symmetries

Proposition A.2 reveals that an additional relationship between H and its adjoint H^* might have important consequences on spectral properties of H. In this subsection, we recall such "symmetry" relations and the corresponding spectral conclusions.

Symmetric operators

A (not necessarily closed) operator H in a Hilbert space $\mathcal{H}$ is said to be *symmetric* if it is densely defined and the adjoint H^* is an extension of H, *i.e.*

$$H^* \supset H\,.$$

A densely defined operator H is symmetric if and only if it is a *formal adjoint* of itself in the sense that $(\phi, H\psi) = (H\phi, \psi)$ for all $\phi, \psi \in \mathsf{D}(H)$, which is equivalent to $\Theta(H) \subset \mathbb{R}$. We say that a symmetric operator H is *non-negative* if $\inf \Theta(H) \ge 0$. If H is symmetric, then the point and continuous spectra of H are real, but the residual spectrum can be complex. (For instance, p^* from Example A.3 considered on a bounded interval or on the half-line is symmetric, but it has complex residual spectra, *cf* Example A.8.) However, if the resolvent set $\rho(H)$ contains at least one real number, then $\sigma(H) \subset \mathbb{R}$.

Self-adjoint operators

If H is densely defined and

$$H^* = H$$

then H is said to be *self-adjoint*. H is automatically closed and has no proper symmetric extensions. With help of the spectral properties of symmetric operators, Proposition A.2 implies that the residual spectrum of self-adjoint operators is empty. Consequently, any self-adjoint operator H satisfies $\sigma(H) \subset \mathbb{R}$. Moreover, the following important identity holds: for every $\lambda \notin \sigma(H)$,

$$\|(H-\lambda)^{-1}\| = \frac{1}{\operatorname{dist}\big(\lambda, \sigma(H)\big)} \,. \tag{A.14}$$

It is usually a straightforward matter to determine whether or not an operator is symmetric, but self-adjointness is a much more delicate property to establish. Regarding our examples, let us mention that the momentum operator from Example A.3 considered in $L^2(\mathbb{R})$ is self-adjoint (so in fact $p = p^*$ if $\Omega = \mathbb{R}$); the free Hamiltonian $-\Delta^{\mathbb{R}^d}$ from Example A.5 is self-adjoint, so are the Dirichlet Laplacian $-\Delta_D^\Omega$, the Neumann Laplacian $-\Delta_N^\Omega$ and the Robin Laplacian $-\Delta_\alpha^\Omega$ if α is real-valued; the operator of multiplication M_V by a function V from Example A.2 is self-adjoint if and only if V is real-valued; finally, iH_0, where H_0 is the generator of the wave equation without damping ($a = 0$) from Example A.14, is self-adjoint.

By one of von Neumann's axioms, physical observables are represented by self-adjoint operators in quantum mechanics. Contrary to what one can occasionally read in a physical literature, this is not just a mathematical laziness, to have real spectra for free (and thus real-valued outcomes of measurement), but it is in fact required by the conservative nature of the theory itself. Indeed, by Stone's theorem, there is a one-to-one correspondence between self-adjoint operators H and strongly continuous one-parameter unitary groups e^{itH} (that determine the time evolution in quantum mechanics).

Normal operators

An operator H is said to be *normal* if it is closed, densely defined and

$$H^*H = HH^* \,,$$

i.e. H commutes with its adjoint H^*. Self-adjoint operators are special cases of normal operators. By the spectral theorem, functions of self-adjoint operators H are normal (including the unitary group e^{itH} and the resolvent $(H-\lambda)^{-1}$ with $\Im\lambda \neq 0$). Normal operators can have complex spectra, but the residual spectrum is again empty. This follows from Proposition A.2 and the property $\mathsf{N}(H) = \mathsf{N}(H^*)$ for any normal operator H. Identity (A.14) holds for normal operators as well.

Example A.15 (Laplacians arising from momentum operators)**.** Let p and p^* be the momentum operators of Example A.3. In $L^2(\mathbb{R})$, p is self-adjoint and thus normal; in fact, $p^*p = -\Delta^{\mathbb{R}} = pp^*$, where $-\Delta^{\mathbb{R}}$ is the free Hamiltonian of Example A.5. In $L^2(\Omega)$ with an arbitrary interval Ω, we have $pp^* = -\Delta_D^\Omega$ and $p^*p = -\Delta_N^\Omega$.

Complex-self-adjoint operators

We say that H in $\mathcal{H}$ is *complex-self-adjoint* (*with respect to* $\mathcal{J}$) if it is densely defined and there exists an antiunitary operator $\mathcal{J}$ in $\mathcal{H}$ such that

$$H^* = \mathcal{J}H\mathcal{J}^{-1} \,. \tag{A.15}$$

Recall that the *antiunitarity* means that $\mathcal{J} : \mathcal{H} \to \mathcal{H}$ is a bijective operator satisfying $(\mathcal{J}\phi, \mathcal{J}\psi) = (\psi, \phi)$ for any $\phi, \psi \in \mathcal{H}$. (This notion should be compared with *unitarity* for which the inner product is preserved, *i.e.* $(\mathcal{J}\phi, \mathcal{J}\psi) = (\phi, \psi)$). In particular, an antiunitary $\mathcal{J}$ is antilinear (or conjugate-linear) and $\mathcal{J}, \mathcal{J}^{-1}$ are bounded. Any complex-self-adjoint operator is automatically closed, which follows from (A.15) and the closedness of the adjoint. If H is complex-self-adjoint, then λ is an eigenvalue of H (with eigenfunction $\psi \in \mathsf{D}(H)$) if and only if $\overline{\lambda}$ is an eigenvalue of H^* (with eigenfunction $\mathcal{J}^{-1}\psi \in \mathsf{D}(H^*)$); consequently, by Proposition A.2,

$$\sigma_{\mathrm{r}}(H) = \varnothing.$$

Example A.16 (Time-reversal operators)**.** A simple example of an antiunitary operator in any Lebesgue space $L^2(\Omega)$ is the complex conjugation $\mathcal{T}\psi := \overline{\psi}$. $\mathcal{T}$ represents a *time-reversal* symmetry operation for a scalar (*i.e.* spinless) Schrödinger equation in $L^2(\mathbb{R}^d)$. For fermionic systems (*i.e.* half-integer non-zero spin), the time-evolution is described by a Pauli equation in the spinorial Hilbert space $L^2(\mathbb{R}^d) \otimes \mathbb{C}^2$, where the time-reversal operator can be represented by the antiunitary operator $\mathcal{T}_{1/2} := \left(\begin{smallmatrix} 0 & \mathcal{T} \\ -\mathcal{T} & 0 \end{smallmatrix}\right)$. Note that $\mathcal{T}^2 = 1$, while $\mathcal{T}_{1/2}^2 = -1$, *cf* [37]. The imaginary Airy operator H_{Airy} from Example A.12 as well as the imaginary cubic oscillator H_{cubic} from Example A.13 are complex-self-adjoint with respect to $\mathcal{T}$. It is easily seen by formal manipulations, but a rigorous verification requires a somewhat more effort since the description of the domain of the adjoint operator is needed; see Theorem A.2 below.

Complex-self-adjoint operators with respect to $\mathcal{J}$ that is involutive (*i.e.* $\mathcal{J}^2 = I$) are sometimes called *$\mathcal{J}$-self-adjoint* [31, Sec. I.4], [23, Sec. III.5] or (somewhat confusingly) *$\mathcal{J}$-symmetric* or *complex symmetric* [27, 28, 50]. For a recent review on this special class of complex-self-adjoint operators with many references we refer to [26].

Pseudo-self-adjoint operators

We say that an operator H in $\mathcal{H}$ is *pseudo-self-adjoint* (*with respect to* G) if H is densely defined and there exists a self-adjoint operator $G \in \mathscr{B}(\mathcal{H})$ with $G^{-1} \in \mathscr{B}(\mathcal{H})$ such that

$$H^* = GHG^{-1}. \tag{A.16}$$

The crucial difference with respect to the notion of complex-self-adjoint operators is that G is assumed to be *linear*. In general, G is indefinite; the case of positive G is very special and will be discussed in more detail in Section A.5.2.

Any pseudo-self-adjoint operator is closed, the reasoning is the same as for complex-self-adjoint operators. Relation (A.16) and Proposition A.2 imply symmetries of the spectra between H and H^*:

$$\sigma_\iota(H) = \sigma_\iota(H^*)\,, \qquad \iota \in \{\mathrm{p}, \mathrm{c}, \mathrm{r}\}\,. \tag{A.17}$$

Contrary to complex-self-adjoint operators, pseudo-self-adjoint operators may have a non-empty residual spectrum (*cf* Example A.18).

Example A.17 (Parity operator)**.** A simple example of an indefinite operator G in $L^2(\mathbb{R}^d)$ is the *parity* (or *space-reversal*) operator $(\mathcal{P}\psi)(x) := \psi(-x)$, which represents a space-reversal symmetry operation in quantum mechanics. The imaginary Airy operator H_{Airy} from Example A.12 as well as the imaginary cubic oscillator H_{cubic} from Example A.13 are pseudo-self-adjoint with respect to $\mathcal{P}$; similarly to the complex-self-adjointness, the proof of this fact is not immediate.

Example A.18 (Shifts on a lattice and perturbations)**.** Let $\mathcal{L}$ be the *left shift* operator in $l^2(\mathbb{Z})$ defined by $\mathcal{L}e_j := e_{j-1}$, where $e_j := (\delta_{kj})_{k\in\mathbb{Z}}$ is the canonical basis in $l^2(\mathbb{Z})$. $\mathcal{L}$ is a unitary operator on $l^2(\mathbb{Z})$ and its adjoint is the *right shift* operator $\mathcal{R}e_j := e_{j+1}$, *i.e.* $\mathcal{L}^* = \mathcal{R}$. The spectrum of $\mathcal{L}$ is discussed in Example A.32. The discrete parity $\mathcal{P}e_j := e_{-j}$ plays the role of an involutive G in this example. It is easy to verify that $\mathcal{L}$ is pseudo-self-adjoint with respect to $\mathcal{P}$.

As a perturbation, let us consider the operator

$$V := -e_0(e_1,\cdot) - e_{-1}(e_0,\cdot) + i\sum_{j=-1}^{-\infty} e_j(e_j,\cdot) - i\sum_{j=1}^{\infty} e_j(e_j,\cdot)\,.$$

Since V is again pseudo-self-adjoint with respect to $\mathcal{P}$, the same holds for the sum $H := \mathcal{L} + V$. Clearly $-i \in \sigma_{\mathrm{p}}(H) = \sigma_{\mathrm{p}}(H^*)$ since e_1 and e_{-1} are the corresponding eigenvectors of H and H^*, respectively. By Proposition A.2, i is either in the point or residual spectrum of H and H^*. We can verify directly that i is not in the point spectrum of H. Indeed,

$$(H-i)\sum_{k\in\mathbb{Z}} \alpha_k e_k = 0 \qquad \Longrightarrow \qquad \begin{cases} \alpha_k = 0, & k \le 0, \\ \alpha_{k+1} = (2i)^k \alpha_1, & k \ge 1, \end{cases}$$

whence $\sum_{k\in\mathbb{Z}} |\alpha_k|^2 = +\infty$, and thus $\mathsf{N}(H-i) = \{0\}$. In summary, H represents a pseudo-self-adjoint operator with non-empty residual spectrum.

If G is indefinite and involutive, the Hilbert space $\mathcal{H}$ equipped additionally to the inner product $(\cdot,\cdot)$ with the *indefinite inner product* $(\cdot, G\cdot)$ is the so-called *Krein space*, *cf* [8, 7]. Then the pseudo-self-adjoint operator H is in fact a self-adjoint operator in this Krein space, *i.e.* H is self-adjoint with respect to the indefinite inner product.

Commutativity

Finally, we discuss a notion which is probably closest to the term "symmetry" in physics. In quantum mechanics, a symmetry operation is represented either by a unitary or antiunitary operator $\mathcal{S}$ in a Hilbert space $\mathcal{H}$. We say that a closed densely defined operator H *has a symmetry* $\mathcal{S}$ if

$$[H, \mathcal{S}] = 0\,, \tag{A.18}$$

i.e. H commutes with $\mathcal{S}$. As usual for the commutativity of an unbounded operator with a bounded operator on $\mathcal{H}$, we understand (A.18) by the operator relation $\mathcal{S}H \subset H\mathcal{S}$. It means that whenever $\psi \in \mathsf{D}(H)$, $\mathcal{S}\psi$ also belongs to $\mathsf{D}(H)$ and $\mathcal{S}H\psi = H\mathcal{S}\psi$.

We also say that H is $\mathcal{S}$*-symmetric*, but this notion should not be confused with $\mathcal{J}$-symmetry or G-symmetry used by other authors in the context of complex-self-adjoint or pseudo-self-adjoint operators, respectively. Finally, we simply say that H *has a symmetry* if there exists a unitary or antiunitary operator $\mathcal{S}$ with respect to which H is $\mathcal{S}$-symmetric.

If the symmetry $\mathcal{S}$ is antiunitary, we deduce from (A.18) that the spectra of H are symmetric with respect to the real axis,

$$(\text{antiunitary symmetry} \Rightarrow) \quad \lambda \in \sigma_\iota(H) \iff \overline{\lambda} \in \sigma_\iota(H)\,,\ \iota \in \{\mathrm{p}, \mathrm{c}, \mathrm{r}\}\,. \tag{A.19}$$

Example A.19 ($\mathcal{PT}$-symmetry)**.** The composition operator $\mathcal{PT}$, where $\mathcal{T}$ is the time-reversal operator from Example A.16 and $\mathcal{P}$ is the space-reversal operator from Example A.17, is the famous (antiunitary) $\mathcal{PT}$*-symmetry*. Both the imaginary Airy operator H_{Airy} from Example A.12 and the imaginary cubic oscillator H_{cubic} from Example A.13 are $\mathcal{PT}$-symmetric. The operator $-\Delta^{(-a,a)}_{\{-i\alpha_0, i\alpha_0\}}$ from Example A.10 is also $\mathcal{PT}$-symmetric.

Non-equivalence of the three operator classes

While the previous examples may suggest that the classes of complex-self-adjoint, pseudo-self-adjoint and those having a symmetry are related, it is not the case in general. Examples of operators with non-empty residual spectrum (*cf* Example A.18 and the right shift on $l^2(\mathbb{N})$ discussed below in this paragraph) show that complex-self-adjoint operators are different from pseudo-self-adjoint operators and from those having an antiunitary symmetry. Moreover, the operator H from Example A.18 is pseudo-self-adjoint, but it cannot have any antiunitary symmetry since it does not satisfy (A.19). Finally, the right shift on $l^2(\mathbb{N})$, *i.e.* the restriction of $\mathcal{R}$ from Example A.18 to $l^2(\mathbb{N})$, has the antiunitary symmetry $\mathcal{T}$ and its residual spectrum is the open unit ball, *cf* [51, Sec.VI.3]. Thus, in view of the Proposition A.2, it cannot satisfy (A.17) and therefore cannot be pseudo-self-adjoint.

A.3 How to whip up a closed operator

In the previous section, we illustrated the abstract notions of spectral theory on concrete examples of differential operators. Since the examples are rather standard, we did not include proofs of closedness. However, our spectral-theoretic approach to non-self-adjoint operators would be incomplete if we did not mention at all how to verify this important property for them. Moreover, in addition to closedness, it is needed that the operator associated with an evolution problem is maximal and quasi-accretive. In the present section, we thus collect some abstract methods which can be effectively used to construct a quasi-m-accretive operator from a formal expression. Again, because of applications, we focus on differential operators, but most of the techniques can be applied more generally.

A.3.1 Closed sectorial forms

Another advantage of m-sectorial operators is that they naturally arise from quadratic forms. Symmetric forms are familiar in quantum mechanics, where they have a physical interpretation of expectation values. For non-self-adjoint operators, a more general class of sectorial forms is needed. Mathematically, the advantage consists in that the theory of forms is simpler than that of operators in several respects.

A *sesquilinear form* (or just *form*) h in a Hilbert space $\mathcal{H}$ is a pair consisting of a linear subspace $\mathsf{D}(h) \subset \mathcal{H}$ called the *domain* of h and a map $h : \mathcal{H} \times \mathcal{H} \to \mathbb{C}$ such that $h(\phi, \psi)$ is linear in $\psi \in \mathsf{D}(h)$ for each fixed $\phi \in \mathsf{D}(h)$ and antilinear in $\phi \in \mathsf{D}(h)$ for each fixed $\psi \in \mathsf{D}(h)$. $h[\psi] := h(\psi, \psi)$ is called the *quadratic form* (or again just *form*) associated with h. We say that h is *densely defined* if $\mathsf{D}(h)$ is dense in $\mathcal{H}$. *Extensions* and *restrictions* of forms are defined in an obvious way as in the case of operators. A form h is said to be *bounded* on $\mathcal{H}$ if there exists a constant $M > 0$ such that $|h[\psi]| \leq M\|\psi\|^2$ for all $\psi \in \mathcal{H}$ and it is *coercive* on $\mathcal{H}$ if there exists a constant $m > 0$ such that $|h[\psi]| \geq m\|\psi\|^2$ for all $\psi \in \mathcal{H}$. The inner product $(\cdot,\cdot)$ is an example of an everywhere defined bounded and coercive sesquilinear form in $\mathcal{H}$ (in fact, $m, M = 1$ in this case).

The *adjoint form* h^* of h is defined in a much simpler way than the adjoint of an operator,

$$h^*(\phi,\psi) := \overline{h(\psi,\phi)}\,, \qquad \mathsf{D}(h^*) := \mathsf{D}(h)\,.$$

We say that h is *symmetric* if $h^* = h$ and there is no notion of "self-adjoint form". The *real* and *imaginary parts* of h are respectively

$$\Re h := \frac{1}{2}(h + h^*)\,, \qquad \Im h := \frac{1}{2i}(h + h^*)\,.$$

This notation is justified by $\Re h[\psi] = \Re(h[\psi])$ and $\Im h[\psi] = \Im(h[\psi])$, although $\Re h(\phi,\psi)$ and $\Im h(\phi,\psi)$ are not real-valued in general and have nothing to do with $\Re(h(\phi,\psi))$ and $\Im(h(\phi,\psi))$.

The *numerical range* of h is defined by

$$\Theta(h) := \{h[\psi] \,:\, \psi \in \mathsf{D}(h),\ \|\psi\| = 1\}\,.$$

As in the case of operators, $\Theta(h)$ is a convex set in the complex plane. Contrary to the case of operators, however, we have a simple relation $\lambda \in \Theta(h) \Leftrightarrow \overline{\lambda} \in \Theta(h^*)$. A form h is symmetric if and only if $\Theta(h) \subset \mathbb{R}$. A symmetric form h is said to be *non-negative* if $\Theta(h) \subset [0,\infty)$.

An important class of forms is given by *sectorial forms* h for which $\Theta(h) \subset S_{\gamma,\vartheta}$, where $S_{\gamma,\vartheta}$ is the sector defined in (A.11) with a vertex $\gamma \in \mathbb{R}$ and a semi-angle $\vartheta \in [0,\pi/2)$. We say that a sectorial form h is *closed* if

$$\left.\begin{aligned} \mathsf{D}(h) \ni \psi_n &\xrightarrow[n\to\infty]{} \psi \in \mathcal{H} \\ h[\psi_n - \psi_m] &\xrightarrow[n,m\to\infty]{} 0 \end{aligned}\right\} \quad \Longrightarrow \quad \big[\psi \in \mathsf{D}(h) \ \wedge \ h[\psi_n - \psi] \xrightarrow[n\to\infty]{} 0\big]\,.$$

If h is sectorial with a vertex $\gamma > -\infty$ and a semi-angle $\vartheta < \pi/2$, then

$$\begin{aligned} |(h-\gamma+1)(\phi,\psi)| &\leq (1+\tan\vartheta)\sqrt{(\Re h - \gamma + 1)[\phi]}\sqrt{(\Re h - \gamma + 1)[\psi]}\,, \\ |(h-\gamma+1)[\psi]| &\geq (\Re h - \gamma + 1)[\psi]\,, \end{aligned}$$

for all $\phi, \psi \in \mathsf{D}(h)$. Consequently, if h is closed, then it is actually bounded and coercive on the Hilbert space $\mathsf{D}(h)$ equipped with the inner product $\Re h(\cdot,\cdot) + (-\gamma+1)(\cdot,\cdot)$. Applying the celebrated Lax-Milgram theorem [23, Sec. IV.1], one can conclude with

Theorem A.1 (First representation theorem)**.** *Let h be a densely defined closed sectorial form in $\mathcal{H}$. Then the operator*

$$\begin{aligned} \mathsf{D}(H) &:= \big\{\psi \in \mathsf{D}(h) \,:\, \exists \eta \in \mathcal{H},\ \forall \phi \in \mathsf{D}(h),\ \ h(\phi,\psi) = (\phi,\eta)\big\}\,, \\ H\psi &:= \eta\,, \end{aligned} \tag{A.20}$$

is m-sectorial.

We say that H is *associated with* h and that $\mathsf{D}(h)$ is the *form-domain* of H. The adjoint of H is simply given by the operator determined by the same theorem with the adjoint form h^*. The numerical range $\Theta(H)$ is a dense subset of $\Theta(h)$. Clearly, $\mathsf{D}(H) \subset \mathsf{D}(h)$ and $h(\phi,\psi) = (\phi, H\psi)$ for every $\phi \in \mathsf{D}(h)$ and $\psi \in \mathsf{D}(H)$ and these conditions determine H uniquely.

Example A.20 (Multiplication operator defined by a sectorial form)**.** If V is the function from Example A.2, we define a quadratic form $m_V[\psi] := \int_\Omega V|\psi|^2$, $\mathsf{D}(m_V) := \{\psi \in L^2(\Omega) : |V|^{1/2}\psi \in L^2(\Omega)\}$. If $V(\Omega) \subset S_{\gamma,\vartheta}$ with $\gamma \in \mathbb{R}$ and $0 \leq \vartheta < \pi/2$, then the multiplication operator M_V from Example A.2 coincides with the m-sectorial operator associated with m_V via Theorem A.1.

A.3.2 Friedrichs' extension

By Theorem A.1, every densely defined closed sectorial form gives rise to an m-sectorial operator. The converse correspondence is also valid. Indeed, if H is m-sectorial, then the form

$$\dot{h}[\psi] := (\psi, H\psi)\,, \qquad \mathsf{D}(\dot{h}) := \mathsf{D}(H)\,, \tag{A.21}$$

is clearly densely defined and sectorial. The form $\dot{h}$ is not necessarily closed, however, it is *closable* in the sense that it admits a closed extension. Then $\dot{h}$ has the *closure* h, *i.e.* the smallest closed extensions, defined by

$$\begin{aligned} \mathsf{D}(h) &:= \left\{\psi \in \mathcal{H} : \exists\{\psi_n\} \subset \mathsf{D}(\dot{h})\,,\ \psi_n \xrightarrow[n\to\infty]{} \psi \ \wedge \ \dot{h}[\psi_n - \psi_m] \xrightarrow[n,m\to\infty]{} 0\right\}, \\ h[\psi] &:= \lim_{n\to\infty} \dot{h}[\psi_n]\,, \end{aligned}$$

and H coincides with the operator associated with h. Summing up, there is a one-to-one correspondence between the set of all m-sectorial operators and the set of all densely defined closed sectorial forms.

Example A.21 (Form associated with a Dirac interaction)**.** The fact that the form $\dot{h}$ defined by (A.21) is closable employs the special structure of its action (*cf* [34, Thm. VI.1.27]). An example of a densely defined sectorial form which is not closable is given by the form associated with the (formal) *Dirac potential* δ in $L^2(\mathbb{R})$: $m_\delta[\psi] := |\psi(0)|^2$, $\mathsf{D}(m_\delta) := H^1(\mathbb{R})$. Note that the form is well defined because of the continuous embedding $H^1(\mathbb{R}) \hookrightarrow C^0(\mathbb{R})$.

The above procedure of constructing a closed form h from a form $\dot{h}$ defined by a sectorial operator H is not limited to closed operators. Indeed, if $\dot{H}$ is just a densely defined sectorial operator, we construct a densely defined sectorial form $\dot{h}$ from it in the same way as in (A.21) (with H being replaced by $\dot{H}$). Then we take the closure h of $\dot{h}$ as above and associate to it the m-sectorial operator H via Theorem A.1. Such a constructed H is called the *Friedrichs extension* of $\dot{H}$.

Any densely defined sectorial operator is *closable* (*i.e.* it admits a closed extension). But there might be many closed extensions and the *closure* (*i.e.* the smallest closed extension) might not be m-sectorial. The importance of the Friedrichs extension lies in the fact that it assigns a special m-sectorial extension to each densely defined sectorial operator. The Friedrichs extension H of $\dot{H}$ is characterised by the properties that, among all m-sectorial extensions of $\dot{H}$, H has the smallest form-domain (*i.e.* $\mathsf{D}(h)$ is contained in the domain of the form associated with any other of the extensions) and that H is the only extension of $\dot{H}$ with $\mathsf{D}(H) \subset \mathsf{D}(h)$.

Example A.22 (The Neumann Laplacian defined by a sectorial form)**.** On the example of the Neumann Laplacian from Example A.5, let us show how to employ the Friedrichs extension in order to construct a closed operator from a formal differential expression. Let $\Omega \subset \mathbb{R}^d$ be an open connected (possibly unbounded) set of class $C^{0,1}$, so that the normal vector $n(x)$ is defined for almost every $x \in \partial\Omega$ by Rademacher's theorem. We start with an operator $\dot{H}$ on $L^2(\Omega)$ that acts as the Neumann Laplacian on nice functions, namely $\dot{H}\psi := -\Delta\psi$, $\mathsf{D}(\dot{H}) := \{\psi \in L^2(\Omega) : \exists\tilde{\psi} \in C_0^\infty(\mathbb{R}^d)$ such that $\psi = \tilde{\psi} \restriction \Omega$ and ψ satisfies (A.5)$\}$. The operator $\dot{H}$ is densely defined and sectorial; in fact, $\dot{H}$ is non-negative due to $(\psi, \dot{H}\psi) = \|\nabla\psi\|^2 \geq 0$ for all $\psi \in \mathsf{D}(\dot{H})$. We define a densely defined sectorial form $\dot{h}$ as in (A.21) (where H is replaced by $\dot{H}$) and construct its closure h. Let H be the m-sectorial operator associated with h via Theorem A.1 (in fact, H is self-adjoint and non-negative). This procedure enable us to define a closed realisation of the Laplacian in Ω, subject to Neumann boundary conditions on $\partial\Omega$, under minimal regularity assumptions on Ω.

Unfortunately, unless we impose some additional restrictions on the boundary $\partial\Omega$, H does not have to coincide with $-\Delta_N^\Omega$ defined in Example A.5 (since $\mathsf{D}(H)$ is not necessarily a subset of $H^2(\Omega)$). Even worse, the boundary condition (A.5) that we understand in the sense of traces of $\psi \in H^2(\Omega)$ might not be well defined. That is, contrary to H, $-\Delta_N^\Omega$ is not well defined under our minimal regularity assumption $C^{0,1}$ on Ω. Let us therefore assume for instance that Ω is bounded and of class C^2; then the boundary traces $H^2(\Omega) \hookrightarrow H^1(\partial\Omega)$ certainly exist [1, Thm. 5.36]. On the other hand, by [14, Thm. 7.2.1], we have $\mathsf{D}(h) = H^1(\Omega)$ (it is remarkable that the boundary condition (A.5) disappears as soon as one passes from the operator $\dot{H}$ to the closure of its quadratic form). From (A.20) we see that $\psi \in \mathsf{D}(H)$ is a solution of the variational problem $(\nabla\phi, \nabla\psi) = (\phi, \eta)$ for every $\phi \in H^1(\Omega)$, which is nothing else than a weak formulation of the Neumann problem $-\Delta\psi = \eta \in L^2(\Omega)$ in Ω, $\partial\psi/\partial n = 0$ on $\partial\Omega$. In particular, $H\psi = -\Delta\psi \in L^2(\Omega)$, where $\Delta\psi$ means the distributional Laplacian of ψ. Using elliptic regularity theory (see, *e.g.*, [12, Thm. 9.26]), we know that the weak solutions ψ belong to $H^2(\Omega)$, which enables us to eventually conclude with $\mathsf{D}(H) = \mathsf{D}(-\Delta_N^\Omega)$. Hence, $H = -\Delta_N^\Omega$, as we wanted to show. In the other extreme situation $\Omega = \mathbb{R}^d$, we verify in the same (in fact easier) manner that $\mathsf{D}(h) = H^1(\mathbb{R}^d)$ and $H = -\Delta_N^{\mathbb{R}^d} = -\Delta^{\mathbb{R}^d}$.

Finally, let us remark that one can introduce the "Neumann Laplacian" for *any* open set Ω by considering the self-adjoint operator associated with the closed form $\tilde{h}[\psi] := \|\psi\|^2$, $\mathsf{D}(\tilde{h}) := H^1(\Omega)$. Again, this definition coincides with $-\Delta_N^\Omega$ from Example A.5 for sufficiently regular Ω.

Example A.23 (The Dirichlet Laplacian defined by a sectorial form)**.** Dirichlet boundary conditions of Example A.5 can be treated in the same way. To get a more robust result, we take the Friedrichs extension H of the operator $\dot{H}\psi := -\Delta\psi$, $\mathsf{D}(\dot{H}) := C_0^\infty(\Omega)$. Then, in the full generality of any open set $\Omega \subset \mathbb{R}^d$, $\mathsf{D}(h) = H_0^1(\Omega)$ and $H\psi = -\Delta\psi$ with $\mathsf{D}(H) = \{\psi \in H_0^1(\Omega) : \Delta\psi \in L^2(\Omega)\}$ is a self-adjoint non-negative operator. If Ω is suficiently regular (*e.g.*, bounded and of class C^2), we obtain $H = -\Delta_D^\Omega$. At the same time, $H = -\Delta_D^{\mathbb{R}^d} = -\Delta^{\mathbb{R}^d}$ if $\Omega = \mathbb{R}^d$.

Robin boundary conditions are best regarded as a perturbation and amenable to the stability methods of Section A.3.4, *cf* Example A.28 below.

A.3.3 M-accretive realisations of Schrödinger operators

The method of quadratic forms does not apply to the more general class of quasi-m-accretive operators. For instance, the imaginary Airy operator from Example A.12 and the imaginary cubic oscillator H_{cubic} from Example A.13 cannot be defined by means of the elegant techniques of Sections A.3.1 and A.3.2. To cover these examples, we present now a specific result obtained by Kato in [36] for Schrödinger operators

$$\mathfrak{H} := -\Delta + V \qquad \text{with} \qquad \Re V \geq 0\,,$$

where $V : \Omega \to \mathbb{C}$ is a function (possibly with singularities). More specifically, we understand $\mathfrak{H}$ as a formal differential expression in an open set $\Omega \subset \mathbb{R}^d$ and are concerned with an m-accretive realisation of $\mathfrak{H}$ that is characterised by Dirichlet boundary conditions. We refer to [23, Sec. VII.2] for a nice exposition of Kato's result and proofs of the present statements.

Assuming

$$V \in L^p_{\text{loc}}(\Omega) \qquad \text{with} \qquad p \begin{cases} = 1 & \text{if} \quad d = 1\,, \\ > 1 & \text{if} \quad d = 2\,, \\ = 2d/(d+2) & \text{if} \quad d \geq 3\,, \end{cases} \tag{A.22}$$

we have $V\psi \in L^1_{\text{loc}}(\Omega)$ for all $\psi \in H^1_0(\Omega)$ and $\mathfrak{H}\psi$ is well defined as a distribution. Then the operator $\tilde{H}\psi := \mathfrak{H}\psi$ with $\mathsf{D}(\tilde{H}) := \{\psi \in H^1_0(\Omega) : \mathfrak{H}\psi \in H^{-1}(\Omega)\}$ is the maximal realisation of $\mathfrak{H}$ as an operator from $H^1_0(\Omega)$ to its dual $H^{-1}(\Omega)$. The message of the following theorem is that the restriction of $\tilde{H}$ to $L^2(\Omega)$ is an m-accretive operator provided that $\Re V \geq 0$ holds.

Theorem A.2 (Kato's theorem)**.** *Let $V : \Omega \to \mathbb{C}$ satisfy* (A.22) *and $\Re V \geq 0$. Then the operator H defined by*

$$H\psi := \mathfrak{H}\psi\,, \qquad \mathsf{D}(H) := \left\{\psi \in H^1_0(\Omega) \,:\, \mathfrak{H}\psi \in L^2(\Omega)\right\} \tag{A.23}$$

is m-accretive in $L^2(\Omega)$. Moreover, the adjoint H^* of H reads

$$H^*\psi = \overline{\mathfrak{H}\overline{\psi}}\,, \qquad \mathsf{D}(H^*) = \left\{\psi \in H^1_0(\Omega) \,:\, \overline{\mathfrak{H}\overline{\psi}} \in L^2(\Omega)\right\}. \tag{A.24}$$

Consequently, H is complex-self-adjoint with respect to the time-reversal operator $\mathcal{T}$ (complex conjugation) introduced in Example A.16. The proof of Theorem A.2 leans heavily on a distributional inequality obtained by Kato in [35], which is an interesting result on its own.

Example A.24 (M-accretivity of the imaginary Airy operator)**.** Function $V(x) := ix$ clearly belongs to $L^\infty_{\text{loc}}(\mathbb{R})$ and satisfies $\Re V \geq 0$, so the operator H defined by Theorem A.2 is m-accretive. We intend to show that H coincides with the operator of H_{Airy} introduced in Example A.12. The inclusion $H_{\text{Airy}} \subset H$ is obvious. To show the opposite one, we employ the fact that H coincides with the closure of $H \restriction C^\infty_0(\mathbb{R})$, *cf* [23, Corol. 2.7]. Hence, $C^\infty_0(\mathbb{R})$ is dense in $\mathsf{D}(H)$ for the graph norm of H. Integrating by parts, we easily check that

$$\begin{aligned} \|\psi'\|^2 &= (\psi, -\psi'') \leq \|\psi\|\|\psi''\| \leq \epsilon\,\|\psi''\|^2 + \epsilon^{-1}\|\psi\|^2\,, \\ \|H\psi\|^2 &= \|\psi''\|^2 + \|x\psi\|^2 + 2\Re(i\psi, \psi') \\ &\geq \|\psi''\|^2 + \|x\psi\|^2 - \epsilon\,\|\psi'\|^2 - \epsilon^{-1}\|\psi\|^2\,, \end{aligned}$$

for every $\psi \in C^\infty_0(\mathbb{R})$ and any $\epsilon > 0$. Combining these inequalities with sufficiently small ϵ and using the density of $C^\infty_0(\mathbb{R})$ in $\mathsf{D}(H)$, we arrive at the non-trivial fact that if $\psi \in \mathsf{D}(H)$, then $\psi \in H^2(\mathbb{R})$ and $x\psi \in L^2(\mathbb{R})$, so $H \subset H_{\text{Airy}}$. Summing up, the m-accretive realisation H obtained by Theorem A.2 coincides with H_{Airy} from Example A.12.

The m-accretivity of the imaginary cubic oscillator from Example A.13 or the self-adjointness of the harmonic oscillator from Example A.4 can be established in the same way.

A.3.4 Small perturbations

Finally, we present two classical perturbation results. If H_0 is a closed operator in $\mathcal{H}$ and V is any operator that belongs to $\mathscr{B}(\mathcal{H})$, then $H_0 + V$ is also closed. For applications, it is necessary to have an extended version of this stability result for a not necessarily bounded perturbation.

Relative boundedness and subordination

Let H_0 and V be two operators in $\mathcal{H}$. We say that V is *relatively bounded* with respect to H_0 if

$$\begin{aligned} &\bullet \quad \mathsf{D}(V) \supset \mathsf{D}(H_0)\,, \\ &\bullet \quad \forall \psi \in \mathsf{D}(H_0)\,, \qquad \|V\psi\| \leq a\,\|H_0\psi\| + b\,\|\psi\|\,, \end{aligned} \tag{A.25}$$

where a, b are non-negative constants. The infimum of such a is called the *relative bound* of V with respect to H_0.

We say that V is *p-subordinated* to H_0 if

$$\begin{aligned} &\bullet \quad \mathsf{D}(V) \supset \mathsf{D}(H_0)\,, \\ &\bullet \quad \forall \psi \in \mathsf{D}(H_0)\,, \qquad \|V\psi\| \leq c\,\|H_0\psi\|^p \|\psi\|^{1-p}\,, \end{aligned} \tag{A.26}$$

where c is a non-negative constant and $p \in [0, 1)$.

Obviously, a bounded V is 0-subordinated to H_0. Moreover, by Young's inequality, any p-subordinated perturbation is relatively bounded with respect to H_0 with the relative bound equal to zero.

Theorem A.3 (Stability of closedness for operators). *If H_0 is closed and V is relatively bounded with respect to H_0 with the relative bound smaller than 1, then $H_0 + V$ is closed.*

The converse is also true: if V is relatively bounded with respect to H_0 with the relative bound smaller than 1 and $H_0 + V$ is not closed, then H_0 cannot be closed.

Example A.25 (Closedness of the generator of the damped wave equation). If H_a is the operator from Example A.14, we write $H_a = H_0 + V$, where $V := \left(\begin{smallmatrix} 0 & 0 \\ 0 & -a \end{smallmatrix}\right)$, $\mathsf{D}(V) := \dot{H}^1_0(\Omega) \times L^2(\Omega)$, is bounded and hence relatively bounded with respect to H_0 with the relative bound equal to zero. At the same time, H_0 is m-accretive because iH_0 is self-adjoint. Therefore, H_a is densely defined and closed for any $a \in L^\infty(\Omega)$. It is m-accretive if $a \leq 0$.

Example A.26 (Shifted harmonic oscillator). When checking that the operator $H_\alpha := p^2 + (q+\alpha)^2$, where p is the momentum operator from Example A.3, q is the position operator from Example A.2 and $\alpha \in \mathbb{C}$, is closed in $L^2(\mathbb{R})$, it helps to regard it as a perturbation of the (self-adjoint) harmonic oscillator H_{HO} from Example A.4. Indeed, estimates analogous to those in Example A.24 yield that the graph norm of H_{HO}, *i.e.* $(\|H_{\mathrm{HO}} \cdot\|^2 + \|\cdot\|^2)^{1/2}$, is equivalent to $(\|\partial_x^2 \cdot\|^2 + \|x^2 \cdot\|^2 + \|\cdot\|^2)^{1/2}$. Then it is easily checked that $H_\alpha := H_{\mathrm{HO}} + V$, where $V := 2\alpha q + \alpha^2$, is $\frac{1}{2}$-subordinated to $H_{\mathrm{HO}} + 1$ and therefore it is also relatively bounded with respect to H_{HO} with the relative bound equal to zero. Applying Theorem A.3, we thus know that H_α is closed on $\mathsf{D}(H_\alpha) = \mathsf{D}(H_{\mathrm{HO}})$.

Relative form-boundedness and subordination

The notion of relative boundedness can be introduced for any forms, but we restrict ourselves to sectorial ones. Let h_0 be a sectorial form in $\mathcal{H}$. A form v in $\mathcal{H}$ (which need not be sectorial) is said to be *relatively bounded* with respect to h_0 if

$$\begin{aligned} &\bullet \quad \mathsf{D}(v) \supset \mathsf{D}(h_0)\,, \\ &\bullet \quad \forall \psi \in \mathsf{D}(h_0)\,, \qquad |v[\psi]| \leq a\,|h_0[\psi]| + b\,\|\psi\|^2\,, \end{aligned} \tag{A.27}$$

where a, b are non-negative constants. Again, the infimum of such a is called the *relative bound* of v with respect to h_0.

A form v in $\mathcal{H}$ is said to be *p-subordinated* to h_0 if

$$\begin{aligned} &\bullet \quad \mathsf{D}(v) \supset \mathsf{D}(h_0)\,, \\ &\bullet \quad \forall \psi \in \mathsf{D}(h_0)\,, \qquad |v[\psi]| \leq c\,|h_0[\psi]|^p \|\psi\|^{2-2p}\,, \end{aligned} \tag{A.28}$$

where c is a non-negative constant and $p \in [0, 1)$.

In parallel to the operator case, the p-subordinated form is also relatively bounded with respect to h_0 with the relative bound equal to zero.

Theorem A.4 (Stability of closedness for forms). *If h_0 is sectorial and closed and v is relatively bounded with respect to h_0 with the relative bound smaller than 1, then $h_0 + v$ is sectorial and closed.*

Again, the converse is also true: if h_0 is sectorial, v is relatively bounded with respect to h_0 with the relative bound smaller than 1 and $h_0 + v$ (which is sectorial) is not closed, then h_0 cannot be closed.

When H_0 is an m-sectorial operator, Theorem A.4 enables one to define operators "$H_0 + V$" even if V has no operator sense. Indeed, the densely defined closed sectorial form h_0 obtained by the closure of (A.21) is associated to H_0 first. Secondly, by Theorem A.4, the sum $h_0 + v$ with a given form v (possibly not arising from an operator or even not closable) is a densely defined closed sectorial form provided that v is relatively bounded with respect to h_0 with the relative bound less than one. Finally, there is an m-sectorial operator associated with $h_0 + v$ via Theorem A.1 (it is sometimes customary to denote this operator by "$H_0 + V$", although the sum may differ from the operator sum).

Example A.27 (Schrödinger operator with a complex Dirac interaction)**.** The Dirac potential (distribution) δ cannot be realised as an operator in $L^2(\mathbb{R})$. However, the Schrödinger operator "$p^2 + \alpha\delta(x)$" with $\alpha \in \mathbb{C}$ can be defined using the strategy of quadratic forms described above. Indeed, $h_0[\psi] := \|\psi'\|^2$, $\mathsf{D}(h_0) := H^1(\mathbb{R})$, is the densely defined closed non-negative form associated with the one-dimensional Laplacian p^2 (*cf* Example A.15 and Example A.22). At the same time, the (non-closable) form m_δ from Example A.21 is $\frac{1}{2}$-subordinated to h_0, and hence relatively bounded with respect to h_0 with the relative bound 0. This follows from the elementary bounds

$$\|\psi\|_\infty^2 \le 2\|\psi\|\|\psi'\| \le \epsilon\,\|\psi'\|^2 + \epsilon^{-1}\,\|\psi\|^2 \tag{A.29}$$

valid for every $\psi \in H^1(\mathbb{R})$ and any $\epsilon > 0$. Hence, by Theorem A.4, the sum $h_0 + \alpha m_\delta$ is a densely defined closed sectorial form to which there exists an m-sectorial operator H_α due to Theorem A.1. H_α can be understood as a form-sum version of "$p^2 + \alpha\delta(x)$". Moreover, with some effort, it is possible to deduce from (A.20) that $(H_\alpha\psi)(x) = -\psi''(x)$ for every $x \neq 0$ and $\mathsf{D}(H_\alpha) = \{\psi \in H^1(\mathbb{R}) \cap H^2(\mathbb{R} \setminus \{0\}) : \psi'(0+) - \psi'(0-) = \alpha\psi(0)\}$.

Example A.28 (The Robin Laplacian defined by a sectorial form)**.** We show that the Robin Laplacian from Example A.5 can be introduced as a perturbation of the Neumann Laplacian. (The resemblance with the preceeding Example A.27 is not accidental.) For simplicity, let us assume that Ω is bounded and of class C^2 and the complex-valued function α belongs to $C^1(\partial\Omega)$. Integrating by parts, we easily check

$$(\psi, -\Delta_\alpha^\Omega\psi) = \int_\Omega |\nabla\psi|^2 + \int_{\partial\Omega} \alpha\,|\psi|^2 =: h_\alpha[\psi]$$

for every $\psi \in \mathsf{D}(-\Delta_\alpha^\Omega)$. However, the right hand side is well defined on a larger space $\mathsf{D}(h_\alpha) := H^1(\Omega)$; indeed the boundary values exist in the sense of the trace embedding $H^1(\Omega) \hookrightarrow L^2(\partial\Omega)$. We write $h_\alpha = h_0 + v$, where $h_0[\psi] := \|\nabla\psi\|^2$ with $\mathsf{D}(h_0) := H^1(\Omega)$ is the form associated with the Neumann Laplacian $-\Delta_N^\Omega$ and $v_\alpha[\psi] := \int_{\partial\Omega} \alpha\,|\psi|^2$ with $\mathsf{D}(v_\alpha) := H^1(\Omega)$ is its perturbation. By Example A.22, h_0 is densely defined, closed and sectorial. To show that v_α is relatively bounded with respect to h_0 (actually $\frac{1}{2}$-subordinated), we estimate the function α by its supremum norm and use the bounds

$$\|\psi\|_{L^2(\partial\Omega)}^2 \le 2\,C\,\|\psi\|\|\nabla\psi\| \le \epsilon\,\|\nabla\psi\|^2 + C^2\epsilon^{-1}\,\|\psi\|^2$$

for every $\psi \in H^1(\Omega)$ and any $\epsilon > 0$, where the constant C depends on curvatures of $\partial\Omega$. (Here the first inequality is actually behind a proof of the trace embedding $H^1(\Omega) \hookrightarrow L^2(\partial\Omega)$.) Hence, by Theorem A.4, the sum h_α is a densely defined closed sectorial form to which there exists an m-sectorial operator H_α due to Theorem A.1. (As a matter of fact, H_α is well defined as an m-sectorial operator for any $\alpha \in L^\infty(\partial\Omega)$.) Continuing as in Example A.22 with help of elliptic regularity theory (for which the extra smoothness of α is needed), one can conclude with $H_\alpha = -\Delta_\alpha^\Omega$.

A.4 Compactness and a spectral life without it

The theory of compact operators in Hilbert spaces is reminiscent of the theory of operators in finite-dimensional spaces. In this section we recall basic properties of this important class of operators and develop a spectral theory for non-compact operators.

A.4.1 Compact operators and compact resolvents

An operator $H \in \mathscr{B}(\mathcal{H})$ is said to be *compact* if, for any bounded sequence $\{\psi_n\} \subset \mathcal{H}$, the sequence $\{H\psi_n\}$ contains a convergent subsequence. Since every bounded sequence in a Hilbert space contains a weakly converging subsequence, the compactness of H means that H maps weakly converging sequences to strongly converging sequences. We denote by $\mathscr{B}_\infty(\mathcal{H})$ the set of all compact operators of $\mathscr{B}(\mathcal{H})$.

Compact operators H have spectacularly nice spectral properties:

- $\sigma(H) \setminus \{0\} = \sigma_{\mathrm{p}}(H) \setminus \{0\}$,
- $\sigma_{\mathrm{p}}(H)$ is at most countable and has no accumulation point except possibly 0,
- $\forall \lambda \in \sigma_{\mathrm{p}}(H) \setminus \{0\}, \quad \mathsf{R}(H-\lambda)$ is closed $\wedge \ \mathsf{m}_{\mathrm{a}}(\lambda) < +\infty$.

That is, every non-zero point λ in the spectrum of a compact operator H is an isolated eigenvalue of finite algebraic multiplicity and the range of $H-\lambda$ is closed. If the Hilbert space $\mathcal{H}$ is infinite-dimensional, zero is always in the spectrum of H, *i.e.* $\sigma(H) = \sigma_{\mathrm{p}}(H) \cup \{0\}$.

Differential operators in $L^2(\Omega)$ are unbounded, so they cannot be compact. However, inverses of differential operators on bounded domains Ω are typically compact. This leads to another important class of operators which have spectra analogous to the spectra of operators in finite-dimensional spaces. We say that a closed operator H in $\mathcal{H}$ has a *compact resolvent* if

- $\rho(H) \neq \varnothing$,
- $(H-\lambda)^{-1} \in \mathscr{B}_\infty(\mathcal{H})$ for some (and hence all) $\lambda \in \rho(H)$.

By virtue of the spectral properties of compact operators and the spectral mapping theorem [23, Thm. IX.2.3], we know that if H has a compact resolvent, then

$$\sigma(H) = \sigma_{\mathrm{disc}}(H),$$

where $\sigma_{\mathrm{disc}}(H)$ is the *discrete spectrum* of H defined (for any closed operator) by

$$\lambda \in \sigma_{\mathrm{disc}}(H) \quad :\Longleftrightarrow \quad \begin{cases} \bullet \ \ \lambda \in \sigma_{\mathrm{p}}(H), \\ \bullet \ \ \lambda \text{ is isolated (as a point in the spectrum)}, \\ \bullet \ \ \mathsf{m}_{\mathrm{a}}(\lambda) < +\infty, \\ \bullet \ \ \mathsf{R}(H-\lambda) \text{ is closed}. \end{cases} \tag{A.30}$$

Example A.29 (Spectrum of the imaginary Airy operator)**.** The operator H_{Airy} from Example A.12 has a compact resolvent; it follows from Example A.24 and the compactness of the embedding $\mathsf{D}(H_{\mathrm{Airy}}) \hookrightarrow L^2(\mathbb{R})$, where the former space is assumed to be equipped with the graph norm of H_{Airy}. Consequently, the spectrum of H_{Airy} is purely discrete. If there existed a non-zero $\psi \in \mathsf{D}(H_{\mathrm{Airy}})$ and $\lambda \in \mathbb{C}$ such that $H_{\mathrm{Airy}}\psi = \lambda\psi$, then, by shifting $\tau_c : x \mapsto x + c$, the function $\psi_c := \psi \circ \tau_c$ would solve $H_{\mathrm{Airy}}\psi_c = (\lambda - ic)\psi$ with any $c \in \mathbb{C}$ and we would thus have $\sigma(H_{\mathrm{Airy}}) = \sigma_{\mathrm{p}}(H_{\mathrm{Airy}}) = \mathbb{C}$, which contradicts the discreteness of the spectrum. Hence, $\sigma(H_{\mathrm{Airy}}) = \varnothing$.

The compact embedding argument shows that the imaginary cubic oscillator from Example A.13 and the shifted harmonic oscillator from Example A.26 have compact resolvents as well. However, their spectra are not empty. In fact, all eigenvalues of both the operators are real and there are infinitely many of them. While the proof of these facts for the latter operator is rather simple (*e.g.* it follows by solving the spectral problem in terms of special functions), the proof for the former is non-trivial [21, 55, 30].

Example A.30 (Green's function of the Laplacian)**.** The Neumann, Dirichlet and Robin Laplacians in $L^2(\Omega)$ from Example A.5 have compact resolvents provided that Ω is bounded and smooth and α is smooth; it follows from the compactness of the Sobolev embedding $H^1(\Omega) \hookrightarrow L^2(\Omega)$. We have the integral representation

$$\left[(-\Delta_\iota^\Omega - k^2)^{-1}\psi\right](x) = \int_\Omega G_{\iota,k}^\Omega(x,y)\,\psi(y)\,dy,$$

where $\iota \in \{D, N, \alpha\}$ and $k^2 \in \rho(-\Delta_\iota^\Omega)$. The integral kernel G_ι^Ω is sometimes referred to as the *Green function*.

The compactness can be checked by hand for the one-dimensional Laplacians considered in Example A.10, where we have explicit formulae

$$\begin{aligned} G_{D,k}^{(-a,a)}(x,y) &= \frac{-\sin(k(x+a))\,\sin(k(y-a))}{k\sin(2ka)}, \\ G_{N,k}^{(-a,a)}(x,y) &= \frac{-\cos(k(x+a))\,\cos(k(y-a))}{k\sin(2ka)}, \\ G_{\alpha,k}^{(-a,a)}(x,y) &= \frac{-\left[k\cos(k(x+a)) - i\alpha\sin(k(x+a))\right]}{(k^2-\alpha^2)\,k\sin(2ka)} \\ &\qquad \times \left[k\cos(k(y-a)) - i\alpha\sin(k(y-a))\right], \end{aligned}$$

for $x < y$ and the role of x, y should be exchanged for $x > y$.

The compactness of the resolvent of many operators can be proved using stability results, which are parallel to the results on the stability of closedness.

Theorem A.5 (Stability of compact resolvent for operators)**.** *Let H_0 be an m-accretive operator which has a compact resolvent. If V is relatively bounded with respect to H_0 with the relative bound smaller than 1, then $H_0 + V$ has a compact resolvent.*

The assumption on m-accretivity of H_0 is not necessary. However, the condition on the relative bound becomes more complicated otherwise. Namely, the conclusion of the theorem holds if there exists $z \in \rho(H_0)$ such that the inequality

$$a\|H_0(H_0 - z)^{-1}\| + b\|(H_0 - z)^{-1}\| < 1$$

is satisfied, *cf* [34, Thm.IV.3.17], where a and b are the constants appearing in (A.25).

Theorem A.5 provides an alternative proof of the compactness of the resolvent for the shifted oscillator from Example A.26.

Theorem A.6 (Stability of compact resolvent for forms)**.** *Let h_0 be a densely defined, closed, sectorial form with $\Re h_0 \geq 0$ and let the associated m-sectorial operator H_0 have a compact resolvent. If v is relatively bounded with respect to h_0 with the relative bound smaller than* 1*, then the operator associated with $h_0 + v$ has a compact resolvent.*

Example A.31 (Harmonic oscillator with a Dirac interaction)**.** We find an m-sectorial realisation of "$H_{\mathrm{HO}} + \alpha\delta(x)$" with $\alpha \in \mathbb{C}$ via the sum of forms. The harmonic oscillator is associated with the form

$$h_{\mathrm{HO}}[\psi] := \|\psi'\|^2 + \|x\psi\|^2 \,, \qquad \mathsf{D}(h_{\mathrm{HO}}) := \{\psi \in H^1(\mathbb{R}) \,:\, x\psi \in L^2(\mathbb{R})\} \,.$$

The inequality (A.29) shows that the form αm_δ is $\frac{1}{2}$-subordinated to h_{HO}, thus relatively bounded with the relative bound 0. Therefore, by Theorems A.4 and A.6, the form $h_{\mathrm{HO}} + \alpha m_\delta$ determines an m-sectorial operator which has a compact resolvent.

A.4.2 Essential spectra

We define the *essential spectrum* of any closed operator H as the complement of the discrete spectrum defined in (A.30), *i.e.*

$$\sigma_{\mathrm{ess}}(H) := \sigma(H) \setminus \sigma_{\mathrm{disc}}(H) \,. \tag{A.31}$$

There is considerable divergence in the literature concerning the definition of the essential spectrum for non-self-adjoint operators. Our definition is the largest within these and was originally introduced by Browder [13]. It makes the essential spectrum harder to locate, but on the other hand, the remaining discrete eigenvalues have very pleasant properties.

Following [23, Chap. IX] (see also [32]), let us compare our definition of the essential spectrum with the others. We assume that H is closed and recall that the resolvent set can be characterised as

$$\begin{aligned}\rho(H) = \{\, \lambda \in \mathbb{C} : \\ \mathsf{R}(H - \lambda) \text{ is closed } \wedge \ \mathsf{nul}(H - \lambda) = 0 = \mathsf{def}(H - \lambda)\} \,.\end{aligned} \tag{A.32}$$

For $k = 0, 1, \ldots, 5$, we set

$$\sigma_{\mathrm{e}k}(H) := \mathbb{C} \setminus \rho_{\mathrm{e}k}(H) \,,$$

where

$$\begin{aligned}
\textit{Goldberg,} \qquad & \rho_{\mathrm{e}0}(H) := \{\lambda \in \mathbb{C} : \mathsf{R}(H - \lambda) \text{ is closed}\} \,, \\
\textit{Kato,} \qquad & \rho_{\mathrm{e}1}(H) := \big\{\lambda \in \rho_{\mathrm{e}0}(H) : \mathsf{nul}(H - \lambda) < \infty \ \vee \ \mathsf{def}(H - \lambda) < \infty\big\} \,, \\
& \rho_{\mathrm{e}2}(H) := \big\{\lambda \in \rho_{\mathrm{e}0}(H) : \mathsf{nul}(H - \lambda) < \infty\big\} \,, \\
\textit{Wolf,} \qquad & \rho_{\mathrm{e}3}(H) := \big\{\lambda \in \rho_{\mathrm{e}0}(H) : \mathsf{nul}(H - \lambda) < \infty \ \wedge \ \mathsf{def}(H - \lambda) < \infty\big\} \,, \\
\textit{Schechter,} \qquad & \rho_{\mathrm{e}4}(H) := \big\{\lambda \in \rho_{\mathrm{e}0}(H) : \mathsf{nul}(H - \lambda) = \mathsf{def}(H - \lambda) < \infty\big\} \,, \\
\textit{Browder,} \qquad & \rho_{\mathrm{e}5}(H) := \text{union of all the components of } \rho_{\mathrm{e}1}(H) \text{ intersecting } \rho(H) \,.
\end{aligned}$$

Clearly,

$$\rho_{\mathrm{e}0}(H) \supset \rho_{\mathrm{e}1}(H) \supset \rho_{\mathrm{e}2}(H) \supset \rho_{\mathrm{e}3}(H) \supset \rho_{\mathrm{e}4}(H) \supset \rho_{\mathrm{e}5}(H) \supset \rho(H) \,,$$

so $\sigma_{\mathrm{e}0}(H)$ is the most restrictive and $\sigma_{\mathrm{e}5}(H)$ is the widest. The names refer to people who are usually associated with the given definition of the essential spectrum. The set $\sigma_{\mathrm{e}2}(H)$ is called the "continuous spectrum" in [31].

The operator $H - \lambda$ is said to be *normally soluble*, *semi-Fredholm* or *Fredholm* if and only if $\lambda \in \rho_{e0}(H)$, $\lambda \in \rho_{e1}(H)$ or $\lambda \in \rho_{e3}(H)$, respectively. The operator H is normally soluble if and only if $\mathsf{R}(H) = \mathsf{N}(H^*)^\perp$, so the condition $\phi \perp \mathsf{N}(H^*)$ is both necessary and sufficient for the equation $H\psi = \phi$ to have a solution ψ (as in finite-dimensional spaces).

Let us show that our definition (A.31) indeed coincides with $\sigma_{e5}(H)$.

Proposition A.5. *Let H be closed. One has*

$$\sigma_{e5}(H) = \sigma_{\text{ess}}(H) .$$

Proof. The statement is equivalent to showing $\rho_{e5}(H) = \rho(H) \cup \sigma_{\text{disc}}(H)$. The set $\rho_{e1}(H)$ is an open subset of the complex plane and it can be written as the union of countably many components (*i.e.* connected open sets) that we denote by $\triangle_n$, $n \in \mathbb{N}$. Kato [34, Sec. IV.5] shows that $\lambda \mapsto \mathsf{nul}(H-\lambda)$ and $\lambda \mapsto \mathsf{def}(H-\lambda)$ are constant in each $\triangle_n$, save possibly at some isolated values of λ. Denoting by ν_n, μ_n these constant values and by λ_n^j, $j \in \mathbb{N}$, these exceptional points in $\triangle_n$, we have

$$\begin{aligned} &\forall \lambda \in \triangle_n \setminus \{\lambda_n^j\}_{j\in\mathbb{N}} , && \mathsf{nul}(H-\lambda) = \nu_n , && \mathsf{def}(H-\lambda) = \mu_n , \\ &\forall j \in \mathbb{N} , && \mathsf{nul}(H-\lambda_n^j) = \nu_n + r_n^j , && \mathsf{def}(H-\lambda_n^j) = \mu_n + r_n^j , \end{aligned}$$

where $0 < r_n^j < \infty$. If $\triangle_n \cap \rho(H) \neq \varnothing$, then $\nu_n = 0 = \mu_n$ and $\triangle_n$ is a subset of $\rho(H)$ except for the λ_n^j which are isolated eigenvalues of H with finite algebraic multiplicities (r_n^j are their geometric multiplicities). Hence, $\rho_{e5}(H) \subset \rho(H) \cup \sigma_{\text{disc}}(H)$. To prove the converse inclusion, we first note that $\rho(H) \subset \rho_{e5}(H)$ is obvious due to (A.32). Finally, if $\lambda \in \sigma_{\text{disc}}(H)$, then of course $\lambda \in \rho_{e1}(H)$. Since λ is isolated, it must belong to a component $\triangle_n$ with $\nu_n = 0 = \mu_n$. But such a component is a subset of $\rho(H)$ except for the exceptional points, λ being one of them; hence, $\triangle_n \cap \rho(H) \neq \varnothing$. ☐

If H is self-adjoint, the sets $\sigma_{ek}(H)$ with $k = 1, \dots, 5$ are identical and $\sigma_{\text{disc}}(H)$ consists of isolated eigenvalues of finite multiplicity ($\mathsf{m}_a(\lambda) = \mathsf{m}_g(\lambda)$ and $\mathsf{R}(H-\lambda)$ is automatically closed). If H is complex-self-adjoint, the sets $\sigma_{ek}(H)$ with $k = 1, \dots, 4$ are identical. In general, however, the inclusion between the sets may be strict, as the following example shows.

Example A.32 (Shift operator and its compact perturbation)**.** Let $\mathcal{L}$ be the *left shift* in $l^2(\mathbb{Z})$ defined in Example A.18. The operator $\mathcal{L}$ is unitary and

$$\sigma(\mathcal{L}) = \sigma_{e5}(\mathcal{L}) = \partial B_1 ,$$

where $B_1 := \{\lambda \in \mathbb{C} : |\lambda| < 1\}$ is an open unit disc. Let V be the compact (in fact of rank 1) operator in $l^2(\mathbb{Z})$ defined by $V := -e_{-1}(e_0, \cdot)$. The sum $H := \mathcal{L} + V$ belongs to $\mathscr{B}(l^2(\mathbb{Z}))$. It is easily shown (*cf* [23, Ex. IX.2.2]) that

$$\sigma_{e5}(H) \supset B_1 , \qquad \text{while} \qquad \sigma_{e4}(H) \subset \partial B_1 .$$

Hence, $\sigma_{e5}(H) \neq \sigma_{e4}(H)$ and $\sigma_{e5}(\mathcal{L})$ is not preserved by the compact perturbation V.

Fortunately, there is a simple way how to exclude pathological situations of the type we encountered in the precedent example.

Proposition A.6. *Let H be closed. If each component of $\rho_{e1}(H)$ intersects $\rho(H)$, then the sets $\sigma_{ek}(H)$ with $k = 1, \dots, 5$ are identical. In particular, the conclusion holds if $\rho_{e1}(H)$ is connected.*

Proof. The result follows at once from the definition of $\rho_{e5}(H)$. ☐

As far as we know, σ_{e2} is associated with no name, but it is useful because of the following characterisation. Although it resembles Weyl's criterion for self-adjoint operators, its proof is quite different (*cf* [63]).

Theorem A.7 (Weyl's criterion)**.** *Let H be a closed and densely defined operator in $\mathcal{H}$. Then*

$$\lambda \in \sigma_{e2}(H) \qquad \Longleftrightarrow \qquad \exists \{\psi_n\}_{n\in\mathbb{N}} \subset \mathsf{D}(H) , \quad \begin{cases} \bullet \quad \forall n \in \mathbb{N} , \quad \|\psi_n\| = 1 , \\ \bullet \quad \psi_n \xrightarrow[n\to\infty]{w} 0 , \\ \bullet \quad (H-\lambda)\psi_n \xrightarrow[n\to\infty]{s} 0 . \end{cases}$$

The sequence from the theorem is called a *singular sequence.*

A.4.3 Stability of the essential spectra

In applications, it often happens that the operator H of interest is obtained from a simpler operator H_0 by a "small" perturbation V, say $H = H_0 + V$. If the essential spectrum of H_0 is easy to locate for some reason, it is of great interest to have criteria on the "smallness" of V which ensure that H and H_0 have the same essential spectrum. By a celebrated result of Weyl, it happens if V is compact. More generally, it is enough to assume that V is "relatively compact" with respect to H_0. Instead of introducing the notion of relative compactness, we state the Weyl's result in the following form (*cf* [23, Thm. IX.2.4]).

Theorem A.8 (Weyl's theorem)**.** *Let H_1, H_2 be closed operators in $\mathcal{H}$ such that*

$$\exists\lambda \in \rho(H_1) \cap \rho(H_2)\,, \qquad (H_1 - \lambda)^{-1} - (H_2 - \lambda)^{-1} \in \mathscr{B}_\infty(\mathcal{H})\,. \tag{A.33}$$

Then

$$\sigma_{\mathrm{e}k}(H_1) = \sigma_{\mathrm{e}k}(H_2) \qquad \text{for} \qquad k = 1, \dots, 4.$$

Unfortunately, the theorem does not apply to our definition of essential spectrum (A.31), which coincides with $\sigma_{\mathrm{e}5}$ by Proposition A.5. In fact, the stability result does not hold for our essential spectrum in general, as Example A.32 clearly demonstrates. Fortunately, Proposition A.6 enables one to use Theorem A.8 also for $\sigma_{\mathrm{e}5}$ in some situations (*e.g.* Example A.33 below).

The last result we would like to mention is not related to essential spectra, but it may turn out to be useful when locating the (essential) spectrum of the "unperturbed" operator H_0 from the opening to this subsection. The following theorem is just [52, Corol. 2 of Thm. XIII.35] translated to the present terminology. Note that the conclusion represents some sort of "separation of variables", which is not at all automatic for non-self-adjoint operators.

Theorem A.9 (Ichinose's lemma)**.** *Let H_1, H_2 be m-sectorial operators in Hilbert spaces $\mathcal{H}_1, \mathcal{H}_2$. Let H denotes the closure of $H_1 \otimes I + I \otimes H_2$ on $\mathsf{D}(H_1) \otimes \mathsf{D}(H_2) \subset \mathcal{H}_1 \otimes \mathcal{H}_2$. Then H is m-sectorial and*

$$\sigma(H) = \sigma(H_1) + \sigma(H_2)\,.$$

Example A.33 ($\mathcal{PT}$-symmetric waveguide)**.** Let $H_{\alpha_0+\beta} := -\Delta_\alpha^\Omega$ be the Robin Laplacian in $L^2(\Omega)$ from Example A.5 with $\Omega := \mathbb{R} \times (-a, a)$, $a > 0$, and $\alpha := \pm i(\alpha_0 + \beta)$ on $\mathbb{R} \times \{\pm a\}$, where α_0 is a real number and β can be identified with a function $\beta : \mathbb{R} \to \mathbb{R}$ that we suppose to be smooth and compactly supported. It is shown in [10] that $H_{\alpha_0+\beta}$ is m-sectorial (the proof is analogous to that given in Example A.28, but notice that Ω is unbounded now). Moreover, $H_{\alpha_0+\beta}$ is easily seen to be complex-self-adjoint with respect to $\mathcal{T}$ and $\mathcal{PT}$-symmetric, where $\mathcal{T}$ is the complex conjugation (*cf* Example A.16) and $(\mathcal{P}\psi)(x_1, x_2) := \psi(x_1, -x_2)$.

The operator $H_{\alpha_0+\beta}$ can be considered as obtained from H_{α_0} by a "small" perturbation. More specifically, the form of $H_{\alpha_0+\beta} - H_{\alpha_0}$ is relatively bounded with respect to the sectorial form of H_{α_0} with the relative bound 0. The "unperturbed" operator H_{α_0} admits the decomposition $-\Delta^{\mathbb{R}} \otimes I + I \otimes -\Delta^{(-a,a)}_{\{-i\alpha_0, i\alpha_0\}}$ in $L^2(\Omega) \simeq L^2(\mathbb{R}) \otimes L^2((-a,a))$, where the one-dimensional Laplacians have been introduced in Examples A.5 and A.10. Applying Theorem A.9 (or employing basis properties of the "transverse" Laplacian as in [10]), we get $\sigma(H_{\alpha_0}) = [\mu_0^2, \infty)$, where $\mu_0^2 := \min\{\alpha_0^2, (\pi/2a)^2\}$ is the lowest eigenvalue of the operator $-\Delta^{(-a,a)}_{\{-i\alpha_0, i\alpha_0\}}$.

The spectrum of H_{α_0} is purely essential, because it has no isolated points, *i.e.*, $\sigma(H_{\alpha_0}) = \sigma_{\mathrm{ess}}(H_{\alpha_0})$. It is proved in [10] that (A.33) holds with the operators $H_1 = H_{\alpha_0}$ and $H_2 = H_{\alpha_0+\beta}$. Combining thus Theorem A.8 with Proposition A.6, we conclude with the stability result

$$\sigma_{\mathrm{ess}}(H_{\alpha_0+\beta}) = \sigma_{\mathrm{ess}}(H_{\alpha_0}) = [\mu_0^2, \infty)\,.$$

Note that the essential spectrum is purely real, though the operator $H_{\alpha_0+\beta}$ is not self-adjoint. Sufficient conditions to guarantee the existence of (real) discrete eigenvalues are also established in [10] (see [43] and [11] for further studies of the model).

A.5 Similarity to normal operators

In finite-dimensional Hilbert spaces, every linear operator is similar to a block diagonal Jordan matrix, whose eigenvalues are elementarily computable. Although there is no general replacement of this result in infinite-dimensional Hilbert spaces, the idea of reducing a given operator to a simpler one by a similarity transformation might work in concrete examples. There are certainly many situations of this type in applications, but we focus on conceptually new approach in quantum mechanics that was suggested by physicists in [54]: represent physical observables by (possibly non-self-adjoint!) operators which are merely similar to self-adjoint ones. In the text below and notably in the examples, we argue that the similarity transformations should be necessarily bounded in order to build a consistent quantum mechanics using this unconventional representation.

A.5.1 Similarity transforms

We say that an operator H_1 is *similar* to another operator H_2 (*via a transformation* A) in the same Hilbert space $\mathcal{H}$ if there exists an injective operator $A \in \mathscr{B}(\mathcal{H})$ with $A^{-1} \in \mathscr{B}(\mathcal{H})$ such that

$$H_2 = AH_1A^{-1}\,. \tag{A.34}$$

This notion is a straightforward generalisation of unitary equivalence with which it shares many important properties such as the preservation of the spectrum.

Proposition A.7. *Let H_1 be a closed operator in a Hilbert space $\mathcal{H}$. If H_2 is similar to H_1, then it is closed and*

$$\sigma_\iota(H_2) = \sigma_\iota(H_1)\,, \qquad \textit{where} \qquad \iota \in \{\ ,\mathrm{p},\mathrm{c},\mathrm{r},\mathrm{disc},\mathrm{ess}\}\,.$$

Moreover, if λ is an eigenvalue of H_1 of geometric multiplicity $\mathsf{m}_\mathrm{g}(\lambda)$ and algebraic multiplicity $\mathsf{m}_\mathrm{a}(\lambda)$, then λ is an eigenvalue of H_2 of the same geometric multiplicity $\mathsf{m}_\mathrm{g}(\lambda)$ and algebraic multiplicity $\mathsf{m}_\mathrm{a}(\lambda)$.

Proof. Let A be a similarity transformation establishing (A.34). Since $A, A^{-1} \in \mathscr{B}(\mathcal{H})$, A and A^{-1} are bijective operators on $\mathcal{H}$ and the relation (A.34) yields

$$\begin{aligned} \mathsf{D}(H_2-\lambda) &= A\,\mathsf{D}(H_1-\lambda)\,, \\ \mathsf{R}(H_2-\lambda) &= A\,\mathsf{R}(H_1-\lambda)\,, \\ \mathsf{N}([H_2-\lambda]^n) &= A\,\mathsf{N}([H_1-\lambda]^n)\,, \end{aligned} \tag{A.35}$$

for any $\lambda \in \mathbb{C}$ and $n \in \mathbb{N}$. The closedness of H_2 can be checked by definition by using the first two identities with $\lambda = 0$. The spectral equivalences can be deduced from the last two identities in (A.35); in particular,

$$\mathsf{nul}(H_2-\lambda) = \mathsf{nul}(H_1-\lambda)\,, \qquad \mathsf{def}(H_2-\lambda) = \mathsf{def}(H_1-\lambda)\,,$$

for any $\lambda \in \mathbb{C}$. We leave the details to the reader. $\square$

Similarity is sometimes understood in a weaker sense, *e.g.* as $AH_1 = H_2A$ without boundedness and invertibility assumptions on A or even as $AH_1\psi = H_2A\psi$ valid for all ψ from a subspace of $\mathcal{H}$ only. The differences in the notions are not always reflected in the terminology. If the assumptions on A are relaxed, many pathologies may occur, particularly the spectra may not be preserved, as the following example demonstrates.

Example A.34 (Gauged and rotated oscillators)**.** A formal (unbounded) similarity transform of the harmonic oscillator leads to the *gauged* (or *Swanson's* [5, 59]) oscillator. For $\phi \in C_0^\infty(\mathbb{R})$, we first define the action of the latter by

$$H_\mathrm{gauged}\phi := (\omega\, a^*a + \alpha\, a^2 + \beta\,(a^*)^2 + \omega)\phi\,, \tag{A.36}$$

where α, β and ω are real parameters such that $\omega \neq \alpha + \beta$, and a^* and a are the creation and annihilation operators from Example A.4. Defining $A := \exp\left(\frac{\beta-\alpha}{\omega-\alpha-\beta}\,\frac{x^2}{2}\right)$, we can easily check that

$$AH_\mathrm{gauged}A^{-1}\phi = \left[(\omega-\alpha-\beta)p^2 + \frac{\omega^2-4\alpha\beta}{\omega-\alpha-\beta}\;q^2\right]\phi =: \tilde{H}_\mathrm{HO}\phi \tag{A.37}$$

for every $\phi \in C_0^\infty(\mathbb{R})$, where the right hand side is just the action of a multiple of the self-adjoint harmonic oscillator with a frequency depending on ω, α and β. In spite of the fact that A or A^{-1} are always unbounded as multiplication operators in $L^2(\mathbb{R})$, equality (A.37) can be read as a weak version of the similarity relation (A.34).

Setting parameters to $\omega = \beta = 0$ and $\alpha = -1$, we thus get an uninteresting "similarity" relation between $-a^2$ and p^2, which are clearly completely different operators. For instance, recalling Examples A.8 and A.9, $\sigma(-a^2) = \sigma_\mathrm{p}(-a^2) = \mathbb{C}$ versus $\sigma(p^2) = \sigma_\mathrm{c}(p^2) = [0,\infty)$. As shown in [49, 41], similar pathologies appear also in less obvious cases, *e.g.* $\omega > 0$, $-\alpha > \omega$, $\beta = 0$, when H_gauged is "highly non-self-adjoint", while $\tilde{H}_\mathrm{HO}$ is still related to the usual harmonic oscillator.

To avoid such pathologies, the parameters need to be restricted by the condition $\omega - |\alpha+\beta| > 0$ as pointed out in [41]. Then H_gauged can be realised as an m-sectorial operator with compact resolvent, for which the spectral equivalence

$$\sigma(H_\mathrm{gauged}) = \sigma(\tilde{H}_\mathrm{HO}) = \left\{(2k+1)\sqrt{\omega^2-4\alpha\beta}\right\}_{k=0}^{\infty}$$

holds. More specifically, H_gauged is defined as the operator in $L^2(\mathbb{R})$ associated with the closed sectorial form

$$\begin{aligned} h_\mathrm{gauged}[\psi] &:= (\omega+\alpha+\beta)\|\psi'\|^2 + (\omega-\alpha-\beta)\|x\psi\|^2 \\ &\qquad + i(\alpha-\beta)\left[(p\psi,x\psi)+(x\psi,p\psi)\right]\,, \\ \mathsf{D}(h_\mathrm{gauged}) &:= \{\psi \in H^1(\mathbb{R}) \,:\, x\psi \in L^2(\mathbb{R})\}\,. \end{aligned}$$

As explained in [41] (*cf* Example A.40 below), the connection between the operators H_{gauged} and $\tilde{H}_{\text{HO}}$ given by (A.37) is very weak, although the operators share the same eigenvalues. Indeed, other important characteristics of H_{gauged}, such as the pseudospectrum and basis properties, are not preserved by the unbounded transformation A. On the other hand, H_{gauged} is *unitarily* equivalent (hence similar according to our restrictive definition) to the *rotated* (or *Davies'* [15]) oscillator

$$\mathcal{U}^* H_{\text{gauged}} \mathcal{U} = \zeta \left(p^2 + \frac{\overline{\zeta}}{\zeta} q^2 \right). \tag{A.38}$$

Here $\zeta := \sqrt{\omega^2 - (\alpha+\beta)^2} + i(\alpha - \beta)$ and $\mathcal{U}$ is a unitary operator with an explicit action (*cf* [41]).

Other warning examples where eigenvalues or other spectral characteristics are not preserved by unbounded similarity transformations can be found in [41]. We do not claim that there are no physical problems where a weaker (*e.g.* unbounded) similarity transformation could be useful (in fact, there are!). However, without the assumption $A, A^{-1} \in \mathscr{B}(\mathcal{H})$, operators H_1 and H_2 cannot be viewed as "equivalent". In particular, H_2 cannot be used as a representation of a self-adjoint observable H_1 in quantum mechanics, unless A and A^{-1} are both bounded.

A.5.2 Quasi-self-adjoint operators

We say that an operator H in a Hilbert space $\mathcal{H}$ is *quasi-self-adjoint* (*with respect to* Θ) if it is densely defined and there exists a non-negative operator $\Theta \in \mathscr{B}(\mathcal{H})$ with $\Theta^{-1} \in \mathscr{B}(\mathcal{H})$ such that

$$H^* = \Theta H \Theta^{-1}. \tag{A.39}$$

That is, H^* is similar to H via the transformation Θ. Self-adjoint operators are quasi-self-adjoint with respect to the identity operator I. More generally, quasi-self-adjoint operators represent a special class of pseudo-self-adjoint operators briefly discussed in Section A.2.5.

Any quasi-self-adjoint operator H is automatically closed, which follows from identity (A.39) and the closedness of the adjoint. In fact, H is self-adjoint with respect to a modified (but topologically equivalent) inner product $(\cdot, \Theta\,\cdot)$ in $\mathcal{H}$. For this reason, the operator Θ is sometimes called a *metric* (it is obviously not unique).

Equivalently, given any decomposition $\Theta = A^*A$, where necessarily $A, A^{-1} \in \mathscr{B}(\mathcal{H})$, H is similar to the operator

$$H_{\text{sa}} := AHA^{-1}, \tag{A.40}$$

which is self-adjoint with respect to the original inner product $(\cdot,\cdot)$ in $\mathcal{H}$. Applying identity (A.14) to H_{sa}, we get

$$\|(H-\lambda)^{-1}\| \le \frac{\kappa}{\operatorname{dist}\big(\lambda, \sigma(H)\big)} \tag{A.41}$$

for every $\lambda \notin \sigma(H)$, where $\kappa := \|A\| \|A^{-1}\|$ is called the *condition number*.

Let us summarise the properties of quasi-self-adjoint operators in the following proposition.

Proposition A.8. *Let H be a densely defined operator in a Hilbert space $\mathcal{H}$. The following statements are equivalent:*

(i) *H is quasi-self-adjoint,*

(ii) *H is similar to a self-adjoint operator.*

Any quasi-self-adjoint operator H is closed, $\sigma(H) \subset \mathbb{R}$, $\sigma_{\text{r}}(H) = \varnothing$ and (A.41) *holds with a constant $\kappa \ge 1$.*

Quasi-self-adjoint operators can be considered as a non-standard (possibly non-self-adjoint) representation of physical observables in quantum mechanics. It is possible to introduce a more general class of "quasi-self-adjoint" operators by relaxing the conditions on the boundedness of Θ and/or Θ^{-1}, *cf* [20]. However, this approach usually leads to pathological situations and does not seem to be adequate for applications in quantum mechanics as argued in [41].

A tool how to prove the quasi-self-adjointness is the following resolvent criterion.

Theorem A.10 ([48, 44, 62])**.** *Let H be a densely defined closed operator in $\mathcal{H}$ with real spectrum. The operator H is similar to a self-adjoint operator if and only if there exists a constant M such that, for every $\psi \in \mathcal{H}$, the two following inequalities*

$$\sup_{\varepsilon>0} \varepsilon \int_{\mathbb{R}} \big\| \big(H - (\xi + i\,\varepsilon)\big)^{-1} \psi \big\|^2 d\xi \le M \|\psi\|^2,$$

$$\sup_{\varepsilon>0} \varepsilon \int_{\mathbb{R}} \big\| \big(H^* - (\xi + i\,\varepsilon)\big)^{-1} \psi \big\|^2 d\xi \le M \|\psi\|^2,$$

are satisfied.

The conditions on the resolvent may be very difficult to verify, unless the resolvent is known explicitly. As an example, let us quote [6], where the conditions are checked for the Laplacian in $L^2(\mathbb{R})$ with point interactions and an explicit formula for the metric is found too. In general, it is not expectable to have closed formulae for the metric operator and similarity transformations, not mentioning the self-adjoint operator to which a given quasi-self-adjoint operator is similar. As another exceptional situation, let us now summarise the complete story about the quasi-self-adjointness of the one-dimensional $\mathcal{PT}$-symmetric Robin Laplacian from Example A.10.

Example A.35 (Quasi-self-adjointness of the complex Robin Laplacian)**.** For the one-dimensional Robin Laplacian $-\Delta^{(-a,a)}_{\{-i\alpha_0,i\alpha_0\}}$ from Example A.10, a metric operator together with the corresponding similarity transformation and the similar self-adjoint operator are known explicitly due to [39, 38, 42]. If $2a\alpha_0/\pi \notin \mathbb{Z}\backslash\{0\}$, the metric Θ and the similarity transform from a decomposition $\Theta = A^*A$ read

$$\Theta = I + K, \quad A = I + L, \quad A^{-1} = I + M, \tag{A.42}$$

where K, L, M are (Hilbert-Schmidt) integral operators with kernels

$$\begin{aligned}
\mathcal{K}(x,y) &:= \alpha_0\, e^{-i\alpha_0(y-x)} \big(\tan(\alpha_0 a) - i\,\mathrm{sgn}(y-x)\big),\\
\mathcal{L}(x,y) &:= \frac{i\alpha_0}{2a}\,\big(y - a\,\mathrm{sgn}(y-x)\big) + \frac{1}{2a}\left(e^{-i\alpha_0(y+a)} - 1\right),\\
\mathcal{M}(x,y) &:= \frac{\alpha_0\, e^{i\alpha_0(a-x)}}{\sin(2\alpha_0 a)} - \frac{\alpha_0}{2}\, e^{-i\alpha_0(x-y)}\big(\cot(2\alpha_0 a) - i\,\mathrm{sgn}(y-x)\big)\\
&\quad - \frac{\alpha_0 e^{-i\alpha_0(x+y)}}{2\sin(2\alpha_0 a)}\,.
\end{aligned}$$

Moreover,

$$A\big(-\Delta^{(-a,a)}_{\{-i\alpha_0,i\alpha_0\}}\big)A^{-1} = -\Delta^{(-a,a)}_N + \alpha_0^2\,\chi_0^N\,(\chi_0^N,\cdot)\,,$$

where $\chi_0^N(x) := (2a)^{-1/2}$ is the first Neumann eigenfunction. The main tool to obtain these formulae is the functional calculus for self-adjoint operators, employing the fact that the eigenfunctions of $-\Delta^{(-a,a)}_{\{-i\alpha_0,i\alpha_0\}}$ can be written down in terms of eigenfunctions of Dirichlet and Neumann Laplacians. We refer [42] for more details and other explicit formulae, even in a more general setting.

Taking the tensor products $I \otimes \Theta$ and $I \otimes A$, $I \otimes A^{-1}$, where I is the identity in $L^2(\mathbb{R})$, we obtain a metric and similarity transformations for the $\mathcal{PT}$-symmetric waveguide H_{α_0} from Example A.33.

A.5.3 Basis properties of eigensystems

In the case of the operators with compact resolvent, the similarity of H to a normal operator is related to the basis properties of the eigenvectors of H. Let us recall some notions first.

We say that $\{\psi_k\}_{k=1}^\infty$ is *complete* in $\mathcal{H}$ if $(\{\psi_k\}_{k=1}^\infty)^\perp = \{0\}$ or equivalently $\mathrm{span}(\{\psi_k\}_{k=1}^\infty)$ is dense in $\mathcal{H}$. We say that $\{\psi_k\}_{k=1}^\infty$ is a *(Schauder or conditional) basis* if every $\psi \in \mathcal{H}$ has a unique expansion in the vectors $\{\psi_k\}$, *i.e.*

$$\forall \psi \in \mathcal{H}, \quad \exists!\{\alpha_k\}_{k=1}^\infty, \quad \psi = \sum_{k=1}^\infty \alpha_k \psi_k\,. \tag{A.43}$$

Finally, we say that $\{\psi_k\}_{k=1}^\infty$, normalised to 1 in $\mathcal{H}$, forms a *Riesz (or unconditional) basis* if it forms a basis and the inequality

$$\forall \psi \in \mathcal{H}, \qquad C^{-1}\|\psi\|^2 \le \sum_{k=1}^\infty |\langle \psi_k, \psi\rangle|^2 \le C\|\psi\|^2 \tag{A.44}$$

holds with a positive constant C independent of ψ. Notice that the Riesz bases are a suitable substitute for orthonormal bases, in which case $C = 1$ due to the Parseval equality. We clearly have

$$\text{complete} \;\supset\; \text{basis} \;\supset\; \text{Riesz basis} \;\supset\; \text{orthonormal basis}\,.$$

A set $\{\psi_k\}_{k=1}^\infty$ is a Riesz basis if there exists an operator $A \in \mathscr{B}(\mathcal{H})$ with $A^{-1} \in \mathscr{B}(\mathcal{H})$ and an orthonormal basis $\{e_k\}_{k=1}^\infty$ such that $e_k = A\psi_k$, see [17, Thm. 3.4.5] for other equivalent formulations. The last property already suggests a relation between the similarity to a normal operator and Riesz basis property, which is expressed more precisely in the following proposition.

Proposition A.9. *Let H have a compact resolvent. Then H is similar to a normal operator if and only if the eigenfunctions of H form a Riesz basis. The latter is equivalent to the similarity to a self-adjoint operator if the spectrum of H is in addition real.*

For non-self-adjoint or non-normal operators, the geometric and algebraic multiplicity of eigenvalues may differ. In that case, the operator cannot be similar to a normal one, nonetheless, the *generalised eigensystem*, *i.e.* the collection of eigenvectors and root vectors, may still contain a Riesz basis. The latter is a suitable generalisation of the similarity to a normal operator and several perturbation results guaranteeing such a property are known. To avoid describing how the root vectors are selected and normalised, the following theorems are expressed with help of spectral projections. We will use the following assumptions and notations in the sequel.

$\langle H_0 \rangle$ Let H_0 be a self-adjoint, non-negative operator which has a compact resolvent. We denote its eigenvalues (sorted in an increasing order) corresponding eigenfunctions and spectral projections as μ_n, ψ_n and P_n, respectively.

Theorem A.11 ([34, Thm. V.4.15a])**.** *Let H_0 satisfy $\langle H_0 \rangle$ above. Assume that all eigenvalues μ_n are simple and*

$$\mu_{n+1} - \mu_n \xrightarrow[n\to\infty]{} \infty \,.$$

Let $V \in \mathscr{B}(\mathcal{H})$ and set $H := H_0 + V$. Then H is closed with compact resolvent, and the eigenvalues and spectral projections of H can be indexed as $\{\lambda_{0k}, \lambda_n\}$ and $\{Q_{0k}, Q_n\}$, respectively, where $k = 1, \dots, N < \infty$ and $n = N+1, N+2, \dots$ in such a way that $|\mu_n - \lambda_n| = O(1)$ as $n \to \infty$ and there exists $A \in \mathscr{B}(\mathcal{H})$ with $A^{-1} \in \mathscr{B}(\mathcal{H})$ such that

$$\sum_{k=1}^{N} Q_{0k} = A^{-1} \sum_{k=1}^{N} P_k A \,, \qquad Q_n = A^{-1} P_n A \,.$$

The claim of this theorem includes the facts that the eigenvalues of the perturbed operator remain simple for $n > N$ and the eigensystem of H contains a Riesz basis composed of eigenvectors of H and finitely many root vectors.

Example A.36 ($\mathcal{PT}$-symmetric square well)**.** We consider a perturbation of the Dirichlet Laplacian $-\Delta_D^{(-a,a)}$ from Example A.10 studied in [65, 57], namely

$$H_Z := -\Delta_D^{(-a,a)} + iZ \operatorname{sgn} x \,, \quad \mathsf{D}(H_Z) := H^2((-a,a)) \cap H_0^1((-a,a)) \,,$$

where Z is a real parameter. Both conditions of Theorem A.11 (*i.e.* the growing gaps of eigenvalues of H_0 and the boundedness of the perturbation) are satisfied, therefore the eigensystem of H_Z contains a Riesz basis for any $Z \in \mathbb{R}$. Since H_Z is $\mathcal{PT}$-symmetric and its eigenvalues depend continuously on Z, all eigenvalues of H_Z are real and simple for all sufficiently small Z and, in this case, H_Z is similar to a self-adjoint operator. When increasing Z, eigenvalues with the lowest real part collide and create complex conjugate pairs. If all eigenvalues of H_Z are simple (some of them possibly complex), then H_Z is similar to a normal operator. For specific values of Z, when two real eigenvalues collide, the geometric multiplicity is one, but the algebraic multiplicity is two, therefore the Riesz basis contains a root vector; in this case, operator H_Z is similar to an "almost diagonal" operator, *i.e.* a two by two Jordan block corresponding to the multiple eigenvalue appears.

Theorem A.11 has many generalisations, using various grow conditions on the eigenvalue gaps and strength of perturbation; we mention particularly classical results in [22] and works using p-subordination, *cf* [64, 45, 4] and references therein. Suitable theorems for perturbations of the harmonic oscillator or similar ones, *i.e.* with asymptotically constant eigenvalue gaps, were proved only recently. We present jointly the operator and form version of the result; further generalisations and related results can be found in [3, 56].

Theorem A.12 ([2, 46])**.** *Let H_0 satisfy $\langle H_0 \rangle$ above. Assume that all eigenvalues μ_n are simple and*

$$\forall n \in \mathbb{N}, \quad \mu_{n+1} - \mu_n \geq \delta > 0.$$

- ***Operator version:*** *Let an operator V, $\mathsf{D}(V) \supset \mathsf{D}(H)$, satisfy*

$$\|V\psi_n\| \xrightarrow[n\to\infty]{} 0 \,. \tag{A.45}$$

Then the claim of Theorem A.11 holds for $H := H_0 + V$.

- ***Form version:*** *Let a sesquilinear form v, $\mathsf{D}(v) \supset \mathsf{D}(h_0)$, satisfy*

$$\forall m, n \in \mathbb{N}, \quad |v(\psi_m, \psi_n)| \leq \frac{M}{m^\alpha n^\alpha}\,, \tag{A.46}$$

  with some $M \geq 0$ and $\alpha > 0$. Then the claim of Theorem A.11 holds for the operator H associated with the sectorial form $h := h_0 + v$, where h_0 is the form associated with H_0.

The classes of potential perturbations of the harmonic oscillator satisfying the conditions (A.45) and (A.46) are studied in [2, 46]; one simple example is the following.

Example A.37 (The eigensystem of the harmonic oscillator with $\alpha\,\delta(x)$)**.** Let H be the operator defined in Example A.31. Since the values of Hermite functions ψ_n, being the eigenfunctions of H_{HO}, at zero are known explicitly, it is not difficult to show that the condition (A.46) is satisfied with $\alpha = 1/4$, *cf* [46]. The latter holds also for perturbations consisting of finitely many δ interactions.

A.6 Pseudospectra

Highly non-self-adjoint operators have properties very different from self-adjoint or normal operators. The notion of pseudospectra is a possibility how to describe these differences and the new phenomena occurring in non-self-adjoint situations. More information on the subject can be found in by now classical monographs by Trefethen and Embree [60] and Davies [17]. Our exposition is in many respects based on [41].

A.6.1 Definition and basic properties

Given a positive number ε, we define the *ε-pseudospectrum* (or simply *pseudospectrum*) of a closed operator H as

$$\sigma_\varepsilon(H) := \left\{ z \in \mathbb{C} \,:\, \|(H-z)^{-1}\| > \varepsilon^{-1} \right\}, \tag{A.47}$$

with the convention that $\|(H-z)^{-1}\| = \infty$ for $z \in \sigma(H)$. Some basic and well-known properties of pseudospectra are summarised in the following:

- *Topology.* For every $\varepsilon > 0$, $\sigma_\varepsilon(H)$ is a non-empty open subset of $\mathbb{C}$ and any bounded connected component of $\sigma_\varepsilon(H)$ has a non-empty intersection with $\sigma(H)$. (If the spectrum of H is empty, then $\sigma_\varepsilon(H)$ is unbounded for every $\varepsilon > 0$.)

- *Relation to spectra.* The pseudospectrum always contains an ε-neighbourhood of the spectrum, and if $\Xi(H)$ defined in (A.9) is connected and has a non-empty intersection with the resolvent set of H, the pseudospectrum is in turn contained in an ε-neighbourhood of the numerical range:

$$\begin{aligned} &\left\{ z \in \mathbb{C} \,:\, \operatorname{dist}\big(z, \sigma(H)\big) < \varepsilon \right\} \subset \sigma_\varepsilon(H) \\ &\qquad\qquad \sigma_\varepsilon(H) \subset \left\{ z \in \mathbb{C} \,:\, \operatorname{dist}\big(z, \overline{\Theta(H)}\big) < \varepsilon \right\}. \end{aligned} \tag{A.48}$$

  The first inclusion follows from the bound $\|(H-z)^{-1}\| \geq \operatorname{dist}\big(z, \sigma(H)\big)^{-1}$, which is valid for any operator. For normal (and thus self-adjoint) operators this inclusion becomes an equality as a consequence of (A.14); hence the notion of pseudospectrum is in fact trivial for such operators. The second inclusion in (A.48) follows from (A.10). If H is "highly non-self-adjoint", the pseudospectrum $\sigma_\varepsilon(H)$ is typically "much larger" than the ε-neighbourhood of the spectrum.

- *Spectral instability.* The following result, sometimes referred to as the Roch-Silberman theorem [53], relates the pseudospectra to the stability of the spectrum under small perturbations:

$$\sigma_\varepsilon(H) = \bigcup_{\|V\| < \varepsilon} \sigma(H + V)\,. \tag{A.49}$$

  This property is of particular importance in applications, for instance in numerical analysis, where small errors (*e.g.* rounding) can easily lead to false identifications of computed eigenvalues of H with possibly very distant eigenvalues of $H + V$ if the pseudospectrum of H is huge.

- *Pseudomodes.* A complex number z belongs to $\sigma_\varepsilon(H)$ if and only if $z \in \sigma(H)$ or z is a *pseudoeigenvalue* (or *approximate eigenvalue*), *i.e.*,

$$\|(H - z)\psi\| < \varepsilon \|\psi\| \quad \text{for some} \quad \psi \in \mathsf{D}(H)\,. \tag{A.50}$$

Any ψ satisfying (A.50) is called a *pseudoeigenvector* (or *pseudoeigenfunction* or *pseudomode*). Again, for operators H which are far from self-adjoint, pseudoeigenvalues may not be close to the spectrum of H. This is particularly striking if we realise that these pseudoeigenvalues can be turned into true eigenvalues by a very small perturbation, *cf* (A.49). What is more, for differential operators, we can often construct very nice (*e.g.* smooth and with compact support) pseudoeigenfunctions, see Section A.6.2.

- *Adjoints.* Using the identity $(H^* - \bar{z})^{-1} = (H - z)^{-1}$ for $z \in \rho(H)$, it is easy to see that

$$\lambda \in \sigma_\varepsilon(H) \iff \overline{\lambda} \in \sigma_\varepsilon(H^*) . \tag{A.51}$$

- *Antiunitary symmetry.* If H has an antiunitary symmetry, *cf* Section A.2.5, then

$$\lambda \in \sigma_\varepsilon(H) \iff \overline{\lambda} \in \sigma_\varepsilon(H) . \tag{A.52}$$

- *Similarity.* If the similarity relation (A.34) holds, then H_1 and H_2 have the same spectra, but their pseudospectra may be very different, unless the condition number κ is fairly close to one since, due to (A.41),

$$\sigma_{\varepsilon/\kappa}(H_2) \subset \sigma_\varepsilon(H_1) \subset \sigma_{\varepsilon\kappa}(H_2) . \tag{A.53}$$

As a consequence, if an operator H_2 is similar to a normal operator H_1, the pseudospectrum of H_1 is contained in the $\varepsilon\kappa$-neighbourhood of $\sigma(H_2)$.

A.6.2 Main tool from microlocal analysis

Pseudospectra of differential operators can be conveniently studied by semiclassical methods, as firstly realised by Davies [16]. His observation was followed by important generalisations, we refer particularly to [66, 19]. In this section we state a simple version of these results adapted to the very special case of differential operators with analytic coefficients in one dimension in a formulation given in [60, Thm. 11.1].

To state the theorem, we need to recall some notions of semiclassical analysis. Let $\hbar > 0$ be a small parameter (inspired by Planck's constant in quantum mechanics; we deliberately avoid frequently used notation h for the small parameter since we reserve this letter for denoting forms) and $a_j : \mathbb{R} \to \mathbb{C}$, with $j = 0, \dots, n$, are smooth functions. Define

$$f(x, \xi) := \sum_{j=0}^{n} a_j(x)(-i\xi)^j , \qquad (x, \xi) \in \mathbb{R}^2 .$$

We say that $H_\hbar$ is a *semiclassical differential operator* associated with *symbol* f if

$$H_\hbar := \sum_{j=0}^{n} a_j(x)\, \hbar^j \, \frac{d^j}{dx^j} , \qquad \mathsf{D}(H_\hbar) := C_0^\infty(\mathbb{R}) . \tag{A.54}$$

The *Poisson bracket* $\{\cdot, \cdot\}$ is defined as

$$\{u, v\} := \frac{\partial u}{\partial \xi}\frac{\partial v}{\partial x} - \frac{\partial u}{\partial x}\frac{\partial v}{\partial \xi} \tag{A.55}$$

and the closure of the set

$$\Lambda := \left\{ f(x, \xi) \,:\, (x, \xi) \in \mathbb{R}^2, \ \frac{1}{2i}\{f, \bar{f}\}(x, \xi) > 0 \right\} \tag{A.56}$$

is referred to as the *semiclassical pseudospectrum* of $H_\hbar$, *cf* [19]. We remark that in the special case of $H_\hbar$ being a Schrödinger operator with analytic potential $a_0 =: V$ the condition $\frac{1}{2i}\{f, \bar{f}\}(x, \xi) > 0$ reduces to $\Im V'(x) \neq 0$ and $\xi \neq 0$.

Now we are in a position to state the result from [60, Thm. 11.1]; we refer to [41] for a proof in the special case of Schrödinger operators.

Theorem A.13 (Semiclassical pseudomodes.)**.** *Let the functions a_j, $j = 0, \dots, n$, be analytic and let $H_\hbar$ be the semiclassical differential operator* (A.54)*. Then, for every $z \in \Lambda$,* cf (A.56)*, there exist $C = C(z) > 1$, $\hbar_0 = \hbar_0(z) > 0$ and an $\hbar$-dependent family of $C_0^\infty(\mathbb{R})$ functions $\{\psi_\hbar\}_{0<\hbar\leq\hbar_0}$ with the property that, for all $0 < \hbar \leq \hbar_0$,*

$$\|(H_\hbar - z)\psi_\hbar\| < C^{-1/\hbar}\, \|\psi_\hbar\|.$$

If the coefficients a_j are not analytic, but only smooth, a slower rate of growth is obtained, *cf* [16, 19]; instead of the upper bound of $C^{-1/\hbar}\|\psi_\hbar\|$ one has that, for each $N \in \mathbb{N}$, there exists a constant $C_N > 0$ such that, for all $0 < \hbar \leq \hbar_0$,

$$\|(H_\hbar - z)\psi_\hbar\| < \frac{\hbar^N}{C_N}\|\psi_\hbar\|.$$

Although Theorem A.13 is stated for semiclassical operators, scaling techniques allow its application to non-semiclassical operators where the spectral parameter tends to infinity. This is based on the principle that the semiclassical limit is equivalent to the high-energy limit after a change of variables; this principle is made concrete in the examples below.

Example A.38 (Pseudospectrum of the imaginary Airy operator)**.** We explain how one can apply Theorem A.13 for the (non-semiclassical) operator H_{Airy} from Example A.12. The scaling argument can be adapted accordingly to the other examples presented below.

We introduce the unitary transform $\mathcal{U}$ on $L^2(\mathbb{R})$ defined by

$$(\mathcal{U}\psi)(x) := \tau^{1/2}\psi(\tau x)\,, \tag{A.57}$$

where $\tau \in \mathbb{R}$ is positive (and typically large in the sequel). Then

$$\mathcal{U}H_{\text{Airy}}\mathcal{U}^{-1} = \tau H_\hbar \quad \text{with} \quad H_\hbar := -\hbar^2\frac{d^2}{dx^2} + ix \quad \text{and} \quad \hbar := \tau^{-3/2}\,.$$

For the symbol $f = \xi^2 + ix$ associated with $H_\hbar$, we have $\{f, \bar{f}\} = -4i\xi$, hence $\Lambda = \{z \in \mathbb{C} : \Re z > 0\}$. The same translation argument which shows that the spectrum is empty, *cf* Example A.29, proves that

$$\|(H_{\text{Airy}} - z)^{-1}\| = \|(H_{\text{Airy}} - \Re z)^{-1}\|.$$

Applying the unitary scaling and Theorem A.13, we know that, for all $\hbar \leq \hbar_0(1)$,

$$\|(H_{\text{Airy}} - \tau)^{-1}\| = \tau^{-1}\|(H_\hbar - 1)^{-1}\| > \hbar^{2/3}C(1)^{1/\hbar}\,.$$

From this we deduce

$$\sigma_\varepsilon(H_{\text{Airy}}) \supset \left\{z \in \mathbb{C} \,:\, \Re z \geq \tau_0 \ \wedge \ (\Re z)^{-1}C(1)^{(\Re z)^{3/2}} \geq \varepsilon^{-1}\right\},$$

where $\tau_0 := \hbar_0(1)^{-2/3}$. Another version of this inclusion is stated in [41, Sec. 7.1]. A quite precise study of the norm of $(H_{\text{Airy}} - z)^{-1}$ as $\Re z \to \infty$ can be found in [9, Cor. 1.4].

Example A.39 (Pseudospectrum of the imaginary cubic oscillator)**.** Now we make a pseudospectral analysis of the paradigmatic $\mathcal{PT}$-symmetric model H_{cubic} from Example A.13. Recall that H_{cubic} has a compact resolvent and that all its eigenvalues are known to be real [21, 55, 30]. On the other hand, its pseudospectrum turns out to be very different from the pseudospectra of self-adjoint operators.

In view of (A.48) and the accretivity of H_{cubic}, we *a priori* know that the pseudospectrum $\sigma_\varepsilon(H_{\text{cubic}})$ is contained in $\{z \in \mathbb{C} : \Re z \geq -\varepsilon\}$. As a consequence of $\mathcal{PT}$-symmetry, we also know that $\sigma_\varepsilon(H_{\text{cubic}})$ is symmetric with respect to the real axis. The unitary transform (A.57) and an application of Theorem A.13 lead to the conclusion that, for every $z \in \Lambda = \{z \in \mathbb{C} : \Re z > 0 \ \wedge \ \Im z \neq 0\}$, there exists $C(z) > 1$ such that, for all $\hbar \leq \hbar_0(z)$,

$$\|(H_{\text{cubic}} - \tau^3 z)^{-1}\| > \hbar^{6/5}C(z)^{1/\hbar}, \quad \hbar := \tau^{-5/2}\,. \tag{A.58}$$

From this we deduce for instance the inclusion

$$\sigma_\varepsilon(H_{\text{cubic}}) \supset \left\{\tau^3 + i\tau^3 \in \mathbb{C} \,:\, \tau \geq \tau_0 \ \wedge \ \tau^{-3}C(1+i)^{\tau^{5/2}} \geq \varepsilon^{-1}\right\},$$

where $\tau_0 := \hbar_0(1+i)^{-2/5}$. We see that, for every ε, there are complex points with positive real part, non-zero imaginary part, and large magnitude that lie in the pseudospectrum $\sigma_\varepsilon(H)$. Consequently, the pseudospectrum of H_{cubic} is not contained in a uniform neighbourhood of $\sigma(H_{\text{cubic}})$, and therefore H_{cubic} is not similar to a self-adjoint operator. From this we also deduce that H_{cubic} is not quasi-self-adjoint (*cf* Proposition A.8) and that its eigenfunctions do not form a Riesz basis (*cf* Proposition A.9).

The asymptotic behaviour of the pseudospectral lines of H_{cubic} is studied in [9, Prop. 4.1], while a result of numerical computations can be found in [60, Fig. 11.4] and [41, Fig. 1], *cf* Figure A.1 below. As the most recent result about H_{cubic}, let us mention [33] where it is shown that the norms of the spectral projections of H_{cubic} grow (at exponential rate), therefore the eigenfunctions cannot form even a basis. Nonetheless, it was proved in [58] that the eigenfunctions are complete.

Example A.40 (Pseudospectrum of the gauged oscillator)**.** In view of Example A.34, the pseudospectrum of the gauged oscillator H_{gauged} (always with $\omega - |\alpha+\beta| > 0$) coincides with the pseudospectrum of a rotated oscillator that appears on the right hand side of (A.38). We could again apply the scaling argument (A.57) and Theorem A.13 to the present situation (see [41, Sec. 7.4]). However, since the pseudospectrum of the rotated oscillator is well studied (see [17] and references therein), we restrict ourselves to saying that it is again much larger than a tubular neighbourhood of the real eigenvalues. Consequently, the rotated oscillator and H_{gauged} are not quasi-self-adjoint and their eigenfunctions do not form a Riesz basis (unless $\alpha = 0 = \beta$). Since it is also known from [18] that the norms of spectral projections grow exponentially, the eigenfunctions do not form even a basis (although they are complete). We refer to [41] for more details on both the pseudospectra and eigenfunctions and for further references.

Let us point out that H_{gauged} satisfies (A.37), which can be interpreted as some sort of weak similarity to the self-adjoint harmonic oscillator H_{HO}. The essential difference in the pseudospectra and basis properties of eigenfunctions of H_{gauged} and H_{HO} clearly demonstrates that the relation (A.37) actually represents only a very weak connection between the two operators.

Example A.41 (Pseudospectrum of the shifted oscillator)**.** Let us consider the shifted harmonic oscillator H_α from Example A.26 with $\alpha = i$. Recall that H_i has a compact resolvent and that all its eigenvalues are real; they actually coincide with the eigenvalues of the self-adjoint oscillator H_{HO} from Example A.4, *cf* Example A.9. Indeed, H_i is *formally* similar to H_{HO} via the *formal* imaginary-shift operator $(A\psi)(x) := \psi(x+i)$.

The pseudospectrum of H_i is symmetric with respect to the real axis as a consequence of $\mathcal{PT}$-symmetry of H_i. Applying the unitary transform (A.57) to the shifted harmonic oscillator H_α from Example A.26 with $\alpha = i$, we end up with an operator of the form

$$\tilde{H}_\hbar := -\hbar^2 p^2 + q^2 + 2i\hbar^{1/2} q - 1\,.$$

Because of the presence of a fractional power of $\hbar$, we do not obtain an operator of the semiclassical type (A.54) and Theorem A.13 is not applicable. Nevertheless, it is still possible to use [16, Thm. 1], which is suitable for potentials with fractional powers of $\hbar$, and thereby obtain polynomial lower bounds to the norm of the resolvent. The expected exponential bound has been proved only recently in [41, Thm. 2] by adapting the proof of Theorem A.13 to the present situation. More specifically, we have

$$\sigma_\varepsilon(H_i) \supset \left\{ z \in \mathbb{C} \,:\, \Re z \geq c^{-1} \ \wedge \ |\Im z| \leq \beta\sqrt{\Re z} \ \wedge \ c e^{c\sqrt{\Re z}} \geq \varepsilon^{-1} \right\},$$

where the number $\beta \in (0,2)$ can be chosen arbitrarily close to 2 and c is a (small) positive constant. Consequently, H_i possesses large complex pseudoeigenvalues in parabolic regions of the complex plane; H_i is not quasi-self-adjoint (*cf* Proposition A.8) and its eigenfunctions do not form a Riesz basis (*cf* Proposition A.9). Summing up, although H_i is formally similar to H_{HO} and their spectra coincide, we see that pseudospectral and basis properties exhibit striking differences.

It has been shown recently in [47] that the eigenfunctions of the shifted oscillator H_i are complete, but do not form a basis since the norms of the spectral projection grow.

Example A.42 (Pseudospectra of the harmonic oscillator with $\alpha\,\delta(x)$)**.** Since the eigensystem of the operator H from Example A.31 form a Riesz basis containing only finitely many root vectors, *cf* Example A.37, H is similar to an operator of the form $D+N$, where D is a diagonal operator having the eigenvalues of H as diagonal entries and N is a finite rank operator corresponding to the Jordan block structure. Standard arguments show that, for z in a neighbourhood of an eigenvalue λ_0 of H, the resolvent satisfies $\|((D+N)-z)^{-1}\| \sim |\lambda_0 - z|^{-n}$, where $n = 1$ if $\mathsf{m}_{\mathrm{a}}(\lambda_0) = \mathsf{m}_{\mathrm{g}}(\lambda_0)$ and $n > 1$ if $\mathsf{m}_{\mathrm{a}}(\lambda_0) > \mathsf{m}_{\mathrm{g}}(\lambda_0)$. The pseudospectrum of H is therefore contained in a neighbourhood of the spectrum, but the possible presence of Jordan blocks results in wider peaks around degenerate eigenvalues with non-equal geometric and algebraic multiplicity.

The same reasoning applies to the $\mathcal{PT}$-symmetric square well from Example A.36.

We refer to [41] for further advocacy of the usage of pseudospectra in non-Hermitian quantum mechanics.

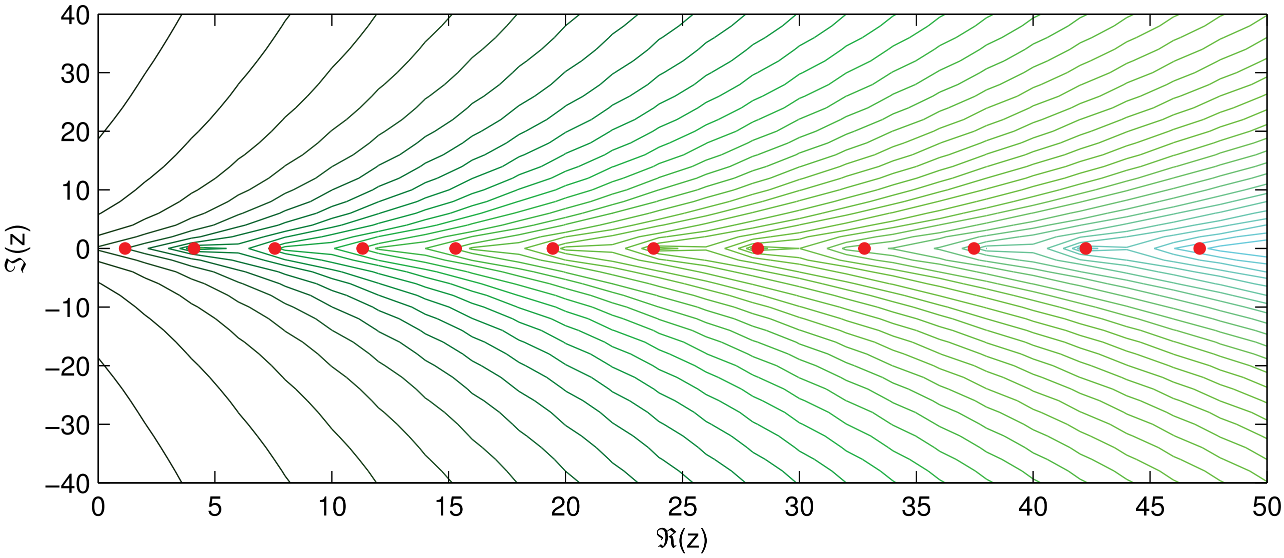

Figure A.1: Spectrum (red dots) and pseudospectra (enclosed by the green contour lines) of the imaginary cubic oscillator. *(Courtesy of Miloš Tater.)*

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$$\|\psi\|^2_{L^2(\partial\Omega)} \leq \epsilon \, \|\nabla\psi\|^2 + C_\epsilon \, \|\psi\|^2 \, ,$$

where the constant C_ϵ depends on ϵ and the geometry of $\partial\Omega$.

Erratum

1. The trace-embedding inequality of Example A.28 should be corrected to

$$\|\psi\|^2_{L^2(\partial\Omega)} \leq \epsilon \, \|\nabla\psi\|^2 + C_\epsilon \, \|\psi\|^2 \, ,$$

where the constant C_ϵ depends on ϵ and the geometry of $\partial\Omega$.

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