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

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September 2017

*Charles University*
*Faculty of Mathematics and Physics*

# Habilitation Thesis

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

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Field:
Mathematics - Mathematical Analysis

Prague 2017

**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.

Prague, Czech Republic
September 2017

*David Krejčiřík*

# 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 $\psi$ 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 $\Theta$ 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 $\Theta$ 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 $\Omega$ 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 $\psi$ 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 $\psi_j$ form a Riesz basis. Denoting by $\phi_j$ 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 $\Theta$ 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 $\Theta$, 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 $\varepsilon$, let us quantify these *spectral instabilities* by introducing the notion of *$\varepsilon$-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 $\varepsilon$-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

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

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 $\varepsilon$,

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

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 $H_\alpha$ 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 $H_\alpha$ 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 $H_\alpha$ well defined as an $m$-sectorial operator with compact resolvent. Consequently, the spectrum of $H_\alpha$ 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 $H_\alpha$ is purely real. However, notice that if $\alpha \in k_1\,\mathbb{Z} \setminus \{0\}$, then $H_\alpha$ admits an eigenvalue of geometric multiplicity one and algebraic multiplicity two (a Jordan block); in this case $H_\alpha$ cannot be similar to a self-adjoint operator. Apart from these exceptional values of $\alpha$, it is shown in [39] that $H_\alpha$ is quasi-self-adjoint. Moreover, using (1.10) and the explicit form of the eigenfunctions (2.3), a closed formula for the metric $\Theta$ 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 $\Theta$ 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 $H_\alpha$ 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 $h_\alpha$ 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 $\alpha$ 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 $h_\alpha$ of $H_\alpha$ 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 $\alpha$ 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 $H_\alpha$ 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, 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 $\Theta$. 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 $\Theta$ (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 $\phi_0$ 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 $\Gamma$ 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 $\psi$ 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 $H_\alpha$ 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 $H_\alpha$ 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 $H_{\alpha_0}$ 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 $H_{\alpha_0}$. Assuming that $\alpha(x)$ tends to a constant $\alpha_0$ as $|x| \to \infty$, we show that the essential spectrum of $H_\alpha$ coincides with the spectrum of $H_{\alpha_0}$. 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 $\varepsilon$, we show that $H_\alpha$ has no eigenvalues converging to $\mu_0^2$ 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 $H_\alpha$ possesses a simple (and therefore real) eigenvalue $\lambda_\varepsilon$ 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 $\varepsilon^3$ as well.

The approach of [11] to the discrete spectrum of $H_\alpha$ 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 $\beta$, 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 $H_\alpha$ by numerical methods. In addition to obtaining a good agreement with the asymptotic formula (2.10), we identify regimes of $\alpha_0$ and $\beta$ 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 $H_\alpha$. 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* $\Sigma$ 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 $\Sigma$ 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 $\kappa$ and $s$ is the curvature and arc-length of $\Sigma$, 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 $\varepsilon$ 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 $\Omega$. 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 $H_\varepsilon$ is non-self-adjoint unless the constants $\alpha_\pm$ are real.

It is natural to expect that $H_\varepsilon$ 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 $H_\varepsilon$ as $\varepsilon \to 0$. We stress that, because of the singular dependence of $H_\varepsilon$ on $\varepsilon$, 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 $\psi$ corresponding to a discrete eigenvalue $\lambda$ 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 $\mathrm{d}_{\mathrm{Ag}}$ 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 $\delta$.

## 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 $\Theta$ such that the weaker quasi-self-adjointness relation (2.8) holds.
2. *The metric is necessarily singular.* That is, no bounded metric operator $\Theta$ 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

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

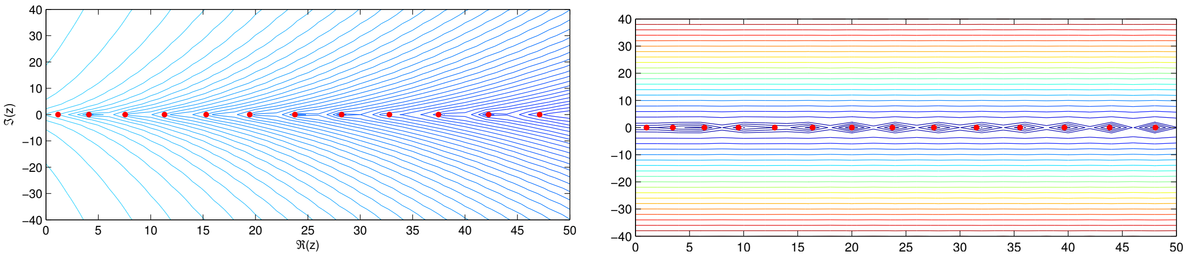
where the first inequality follows from the fact that the spectrum of $H$ is real, the second inequality is due to the assumption that the pseudospectrum of $H$ is trivial, the equality employs the scaling above and the last inequality (the crucial step) follows from known semiclassical results for non-self-adjoint 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 $\varepsilon$. 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 $\varepsilon$-pseudospectrum is just the $\varepsilon$-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 $\mathcal{S}$.

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 $\varepsilon$) for all small $\varepsilon$. 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

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

where the number $z$ and the vector $\psi$ 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 $\varepsilon$).

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 $\psi_k$ 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, $\psi_{-1}$ 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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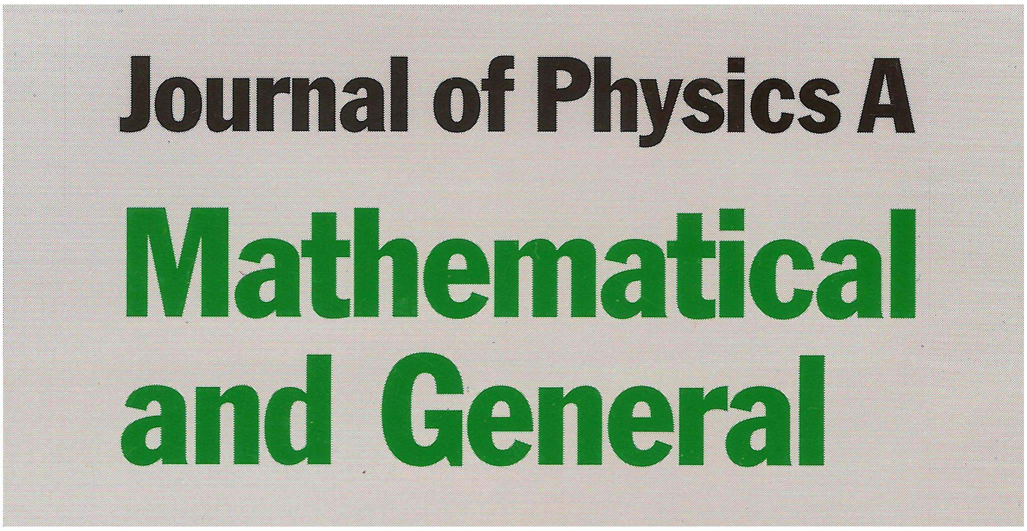
# Part I

# Toy models

# Chapter 3

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




**Published in:** Journal of Physics A: Mathematical and General **39** (2006), 10143–10153
`https://doi.org/10.1088/0305-4470/39/32/S15`

**Joint work with:** Hynek Bíla and Miloslav Znojil

## Chapter 4

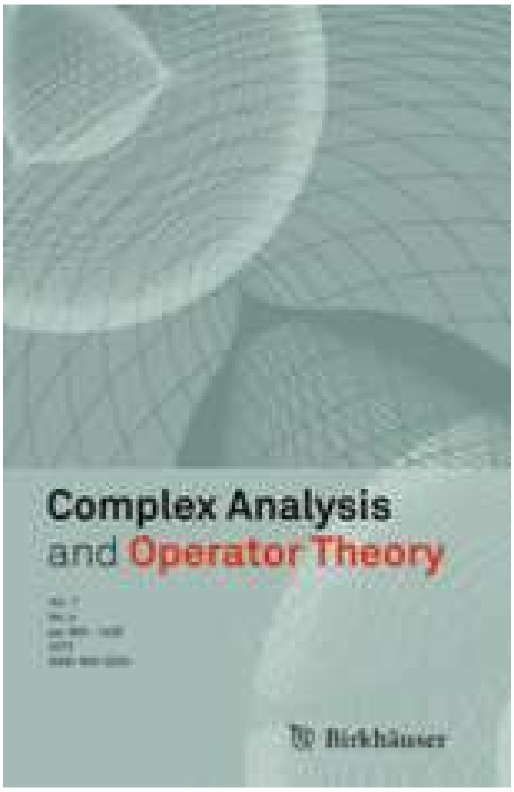
# Calculation of the metric in the Hilbert space of a $\mathcal{PT}$-symmetric model via the spectral theorem

Journal of Physics A
Mathematical and Theoretical

**Published in:** Journal of Physics A: Mathematical and Theoretical **41** (2008) 244012
https://doi.org/10.1088/1751-8113/41/24/244012

## Chapter 5

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




**Published in:** Complex Analysis and Operator Theory **8** (2014), 255–281
https://doi.org/10.1007/s11785-013-0301-y

**Joint work with:** Petr Siegl and Jakub Železný

# Chapter 6

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


**Published in:** Physics Letters A **375** (2011), 2149–2152
`https://doi.org/10.1016/j.physleta.2011.04.021`

**Joint work with:** Hector Hernandez-Coronado and Petr Siegl

# Chapter 7

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

Journal of Physics A
Mathematical and Theoretical

**Published in:** Journal of Physics A: Mathematical and Theoretical **43** (2010) 485204
`https://doi.org/10.1088/1751-8113/43/48/485204`

**Joint work with:** Petr Siegl

# Chapter 8

# The Pauli equation with complex boundary conditions

Journal of Physics A
Mathematical and Theoretical

**Published in:** Journal of Physics A: Mathematical and Theoretical **45** (2012), 444019.
https://doi.org/10.1088/1751-8113/45/44/444019

**Joint work with:** Denis Kochan, Radek Novák and Petr Siegl

# Chapter 9

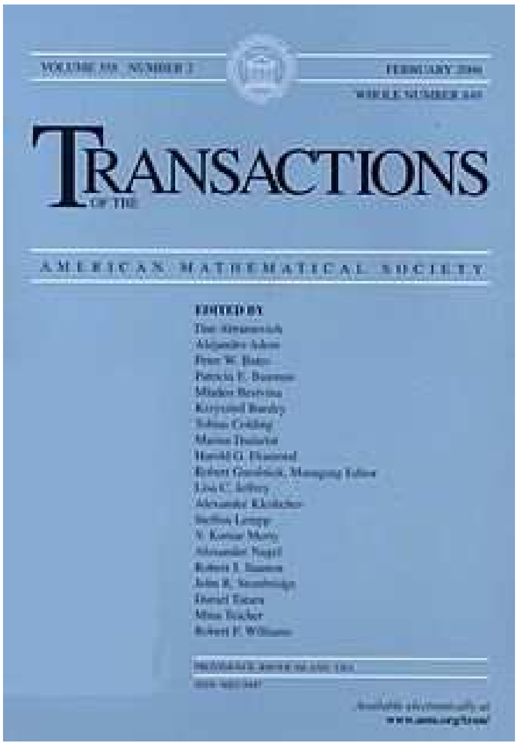
# Spectral analysis of the diffusion operator with random jumps from the boundary


**Published in:** Mathematische Zeitschrift **284** (2016), 877–900
https://doi.org/10.1007/s00209-016-1677-y

**Joint work with:** Martin Kolb

# Chapter 10

# Non-self-adjoint graphs




**Published in:** Transactions of the American Mathematical Society **367** (2015), 2921–2957
`https://doi.org/10.1090/S0002-9947-2014-06432-5`

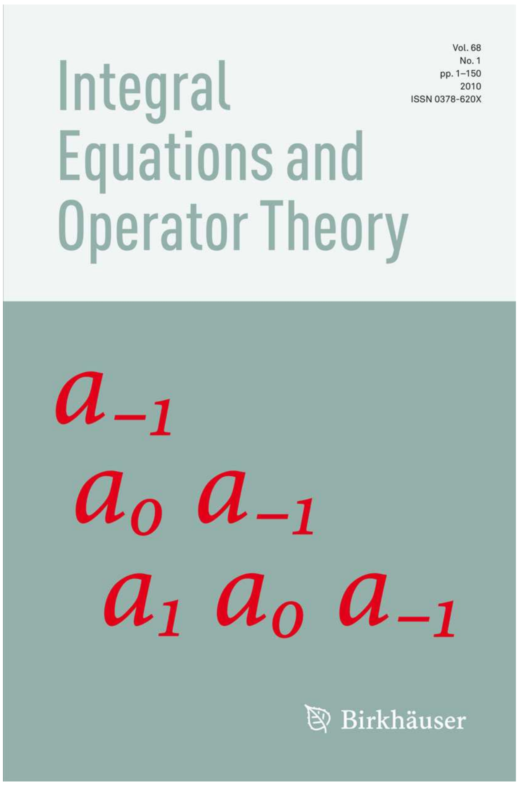
**Joint work with:** Amru Hussein and Petr Siegl

# Part II

# Waveguides

# Chapter 11

# $\mathcal{PT}$-symmetric waveguides




**Published in:** Integral Equations and Operator Theory **62** (2008), 489–515
`https://doi.org/10.1007/s00020-008-1634-1`

**Joint work with:** Denis Borisov

# Chapter 12

# Non-Hermitian spectral effects in a $\mathcal{PT}$-symmetric waveguide

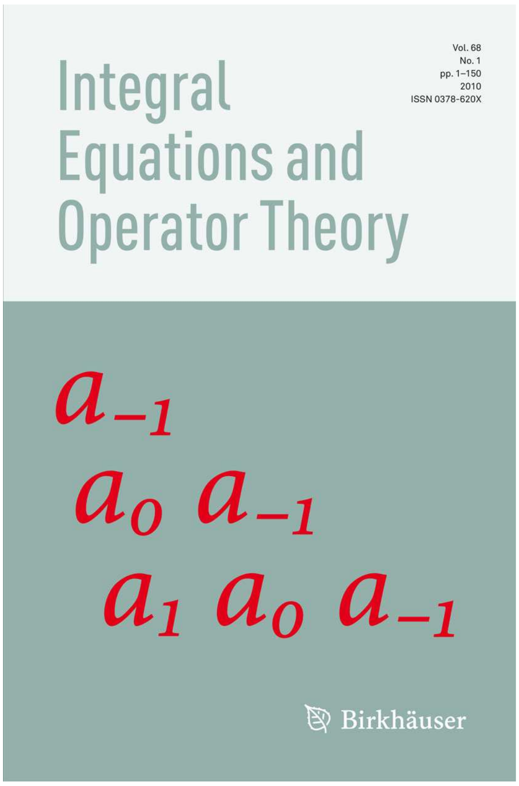
Journal of Physics A
Mathematical and Theoretical

**Published in:** Journal of Physics A: Mathematical and Theoretical **41** (2008) 244013
https://doi.org/10.1088/1751-8113/41/24/244013

**Joint work with:** Miloš Tater

# Chapter 13

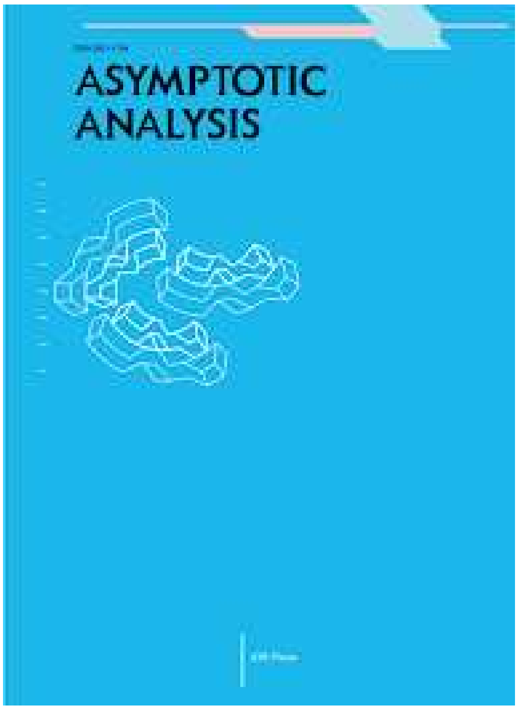
# $\mathcal{PT}$-symmetric waveguides and the lack of variational techniques




**Published in:** Integral Equations and Operator Theory **73** (2012), 1–2
https://doi.org/10.1007/s00020-011-1926-8

# Chapter 14

# The effective Hamiltonian for thin layers with non-Hermitian Robin-type boundary conditions




**Published in:** Asymptotic Analysis **76** (2012), 49–59
`https://doi.org/10.3233/ASY-2011-1061`

**Joint work with:** Denis Borisov

# Chapter 15

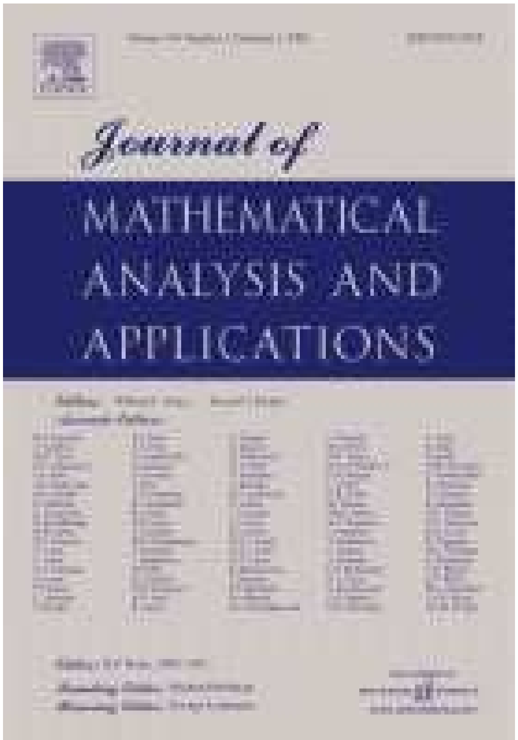
# Reduction of dimension as a consequence of norm-resolvent convergence and applications

**Preprint on:** arXiv:1701.08819 [math-ph] (2017)
`https://arxiv.org/abs/1701.08819`

**Joint work with:** Nicolas Raymond, Julien Royer and Petr Siegl

# Chapter 16

# Asymptotic spectral analysis in colliding leaky quantum layers




**Published in:** Journal of Mathematical Analysis and Applications **446** (2017), 1328–1355
https://doi.org/10.1016/j.jmaa.2016.09.032

**Joint work with:** Sylwia Kondej

# Chapter 17

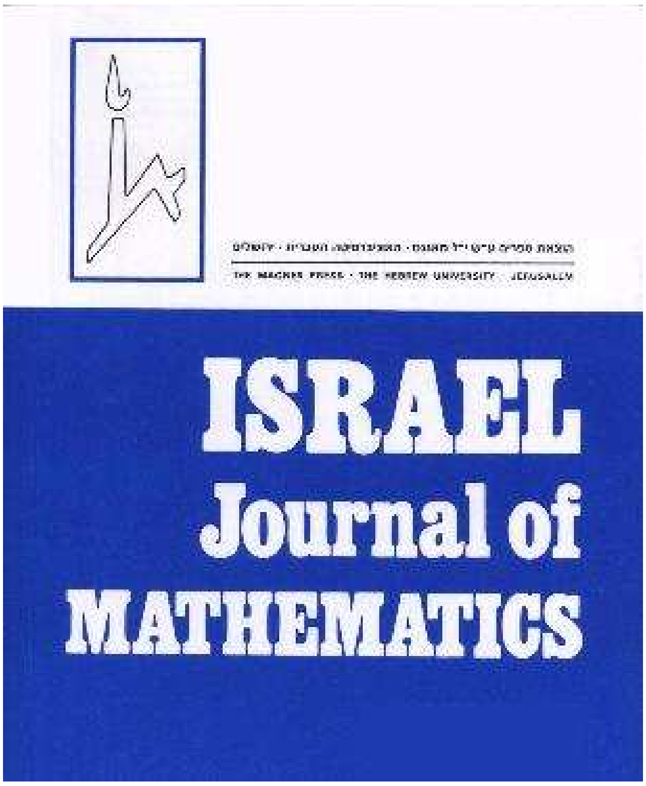
# Spectral stability of Schrödinger operators with subordinated complex potentials


**Published in:** Journal of Spectral Theory, to appear
`https://doi.org/10.4171/JST` (preprint on `http://arxiv.org/abs/1506.01617`)

**Joint work with:** Luca Fanelli and Luis Vega

# Chapter 18

# Non-accretive Schrödinger operators and exponential decay of their eigenfunctions




**Published in:** Israel Journal of Mathematics, to appear
`http://www.ma.huji.ac.il/~ijmath/` (preprint on `http://arxiv.org/abs/1605.02437`)

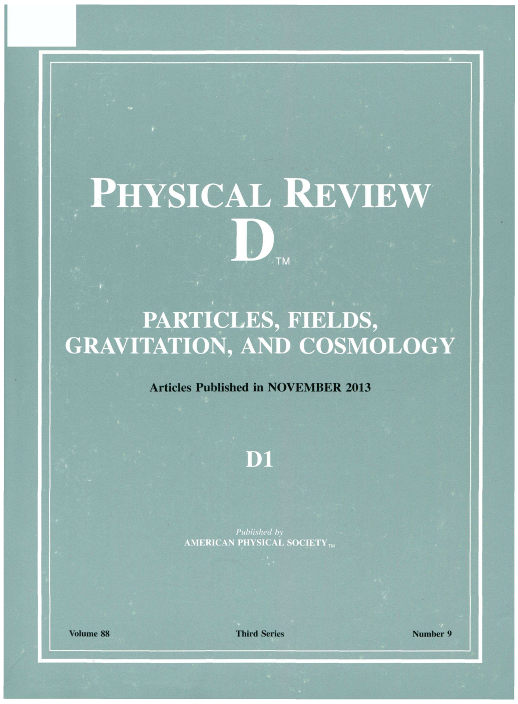
**Joint work with:** Nicolas Raymond, Julien Royer and Petr Siegl

# Part III

# Pseudospectra

# Chapter 19

# On the metric operator for the imaginary cubic oscillator




**Published in:** Physical Review D **86** (2012), 121702(R)
`https://doi.org/10.1103/PhysRevD.86.121702`

**Joint work with:** Petr Siegl

# Chapter 20

# Pseudospectra in non-Hermitian quantum mechanics

**Published in:** Journal of Mathematical Physics **56** (2015), 103513
`http://dx.doi.org/10.1063/1.4934378`

**Joint work with:** Joe Viola, Petr Siegl and Miloš tater

# Chapter 21

# Pseudospectra of the Schrödinger operator with a discontinuous complex potential


**Published in:** Journal of Spectral Theory, to appear
https://doi.org/10.4171/JST (preprint on http://arxiv.org/abs/1503.02478)

**Joint work with:** Raphaël Henry

# Chapter 22

# Pseudomodes for Schrödinger operators with complex potentials

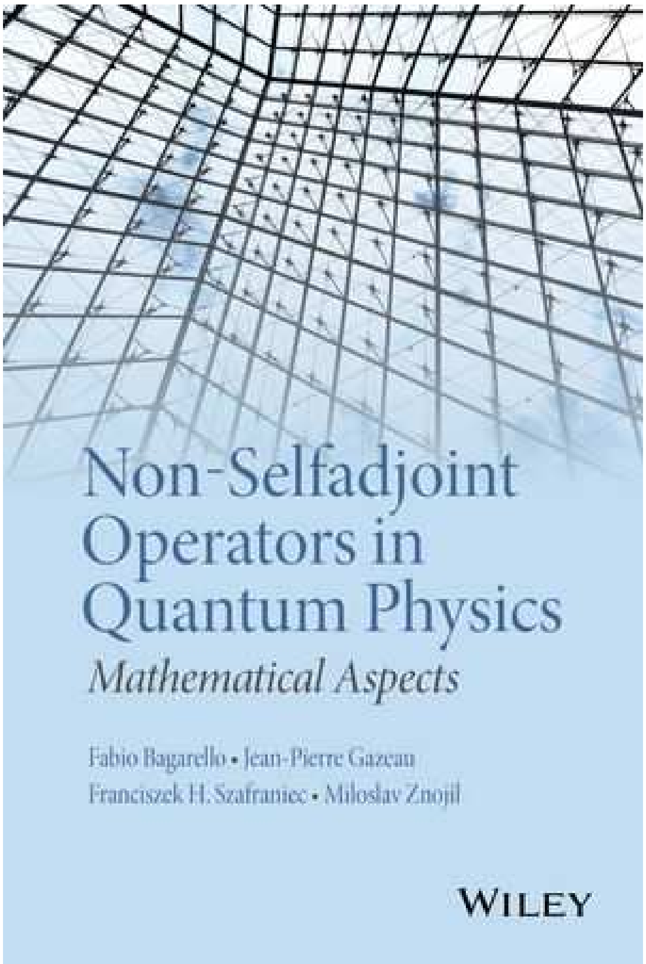
**Preprint on:** arXiv:1705.01894 [math.SP] (2017)
`https://arxiv.org/abs/1705.01894`

**Joint work with:** Petr Siegl

# Appendix

# Appendix A

# Elements of Spectral Theory without the Spectral Theorem




**Published in:** "Non-Selfadjoint Operators in Quantum Physics: Mathematical Aspects",
F. Bagarello, J.-P. Gazeau, F. H. Szafraniec, and M. Znojil, Eds., Wiley-Interscience, 2015
http://dx.doi.org/10.1002/9781118855300

**Joint work with:** Petr Siegl