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Nonstandard perturbation methods and non-Hermitian models in Quantum Mechanics

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Abstrakt

V této dizertaci se zabýváme zkoumáním spectra Schrödingerovských operátorů
$$H = -\Delta + Q(x), \quad L^2(\Omega),$$
kde $\Omega \subset \mathbb{R}^d$ je otevřená s Dirichletovskou hraniční podmínkou na $\partial\Omega$ a $Q : \Omega \to \mathbb{C}$. Studujeme kvantovou mechaniku se samosdruženými, kvazi-samosdruženými a nesamosdruženými pozorovatelnými H. Poruchová teorie a spektrální aproximace jsou hlavními nástroji použitými v této práci. Aproximující operátory se mohou lišit jak v potenciálu, tak v doméně. Asymptotické vzorce vlastních hodnot jsou odvozeny a jejich platnost dokázána pro rozličné problémy se silnou vazbou $Q(x, g)$, $g \to \infty$ a pro divergující vlastní hodnoty, které se objevují při osekávání domén Schrödingerovských operátorů s komplexním potenciálem.

Abstract

This thesis is devoted to investigation of the spectra of Schrödinger operators
$$H = -\Delta + Q(x), \quad L^2(\Omega)$$
with $\Omega \subset \mathbb{R}^d$ open, Dirichlet boundary conditions at $\partial\Omega$ and $Q : \Omega \to \mathbb{C}$. We study quantum mechanics with self-adjoint, quasi-self-adjoint and non-self-adjoint observables H. Perturbation theory and spectral approximations are the main tools used in this thesis. The approximating operators may differ in both potential and domain. Asymptotic formulae for eigenvalues are derived and proven to be true for various problems with strong coupling $Q(x, g)$, $g \to \infty$ and for diverging eigenvalues occuring in domain truncations of Schrödinger operators with complex potential.

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Contents

Introduction

In quantum mechanics, observables are described by linear operators on infinite-dimensional Hilbert spaces, such as $L^2(\Omega)$, $\Omega \subset \mathbb{R}^d$ open, and the measured values of physical quantities such as energy or momentum corresponds to their spectral values. Investigation of their spectra is therefore of major importance. Of particular interest are the spectra of the Hamiltonian

$$H = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + Q(x), \qquad \text{in } L^2(\Omega) \tag{1}$$

with $\Omega \subset \mathbb{R}^d$ open, standing for the total energy of a quantum mechanical system.

Only a few specific choices of Q and Ω, with suitable boundary conditions at $\partial\Omega$, lead to exactly solvable problem, *e.g.* harmonic oscillator $Q(x) = x^2$, $\Omega = \mathbb{R}^d$. In most cases we have to use other tools including perturbation theory and other approximative methods.

In the first chapter 1 we focus on standard quantum mechanics, where the operator (1) is considered self-adjoint. For relatively bounded perturbations of a known problem, *e.g.*

$$-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + g \ln \frac{1}{x^2}, \quad L^2((-1,1)) \tag{2}$$

we can use Rayleigh-Schrödinger perturbation theory, as discussed in Section 1.1. In Section 1.2 we discus operators with strong coupling g in the potential $Q(x,g)$. In special cases, the potential can be linearly or quadraticly approximated. In the quadratic approximation approach, after suitable transformation we discus operators in a form

$$A_g = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + x^2 + R(x,g), \quad L^2(\mathcal{I}_g) \tag{3}$$

with $R(x,g) \to 0$ and $\mathcal{I}_g \to \mathbb{R}$ as $g \to \infty$. In such a scenario A_g contain asymptotically the eigenvalues

$$\lambda_{n,g} = \lambda_n + r_{n,g}, \quad g \to \infty \tag{4}$$

with $r_{n,g} \to 0$ as $g \to \infty$ and $\lambda_n = 2n + 1$. Similarly for linear approximation with λ_n being the eigenvalues of Airy operator defined on $L^2(\mathbb{R}_+)$ and $\mathcal{I}_g \to \mathbb{R}_+$ as $g \to \infty$. By writing that spectra of operators $\{A_g\}$ contain asymptotically the eigenvalues $\{\lambda_{n,g}\}_n$ we mean that

$$\forall g > 0, \quad \exists n_g \in \mathbb{N}, \quad \forall n > n_g, \quad \lambda_{n,g} \in \sigma(A_g). \tag{5}$$

The convergence results for eigenvalues are proven via the notion of pseudospectra and its properties.

Self-adjoint operators are similar to quasi-self-adjoint operators for which Q may be complex. This subclass of non-self-adjoint operators, discussed in Chapter 2, have real spectra so that we can build consistent quantum mechanics with a quasi-self-adjoint observable H. In order to do so, we need a positive, bounded and boundedly invertible metric operator Θ which satisfies

$$H^* = \Theta H \Theta^{-1}. \tag{6}$$

The construction of proper metric operator is a major challenge even for one observable, especially for unbounded operators. In this chapter we consider quantum mechanical system with more than one observable. In such a case, we have to examine the conditions for existence of common metric, which in many cases may not exist at all, as demonstrated on our finite-dimensional example.

We can choose (1) to be non-self-adjoint with $Q : \mathbb{R}^d \to C$. In general, the spectrum of such problem is complex and includes extreme scenarios where $\sigma(H) = \emptyset$ or $\sigma(H) = \mathbb{C}$. Nevertheless, such models are becoming more popular and have applications in physics. In Section 3.4, we are interested in models

$$T_g = -\Delta + Q_1 + \mathrm{i}gQ_2, \quad L^2(\Omega) \tag{7}$$

where $\Omega \subset \mathbb{R}^d$ is open and $Q_i : \Omega \to \mathbb{R}$, $i = 1, 2$ and $g \to \infty$. We use ideas about transformation of operators already used in Chapter 1, but in this scenario we need to use more sophisticated mathematical tools in order to prove the convergence results. Specifically we use resolvent estimates and norm resolvent convergence of a sequence of operators.

In chapter 4 we discus the domain truncation technique, which is very useful to determine the spectra of operators defined on unbounded domains, provided that for given operator such approximation is spectrally exact. In this work we focus our attention on the so called diverging eigenvalues which occur while applying domain truncation technique to non-self-adjoint operators, specifically (1) with $Q(x) = \mathrm{i}U(x)$. *e.g.* the imaginary oscillator

$$T_\infty = -\Delta_{\mathrm{D}} + \mathrm{i}|x|^2 \tag{8}$$

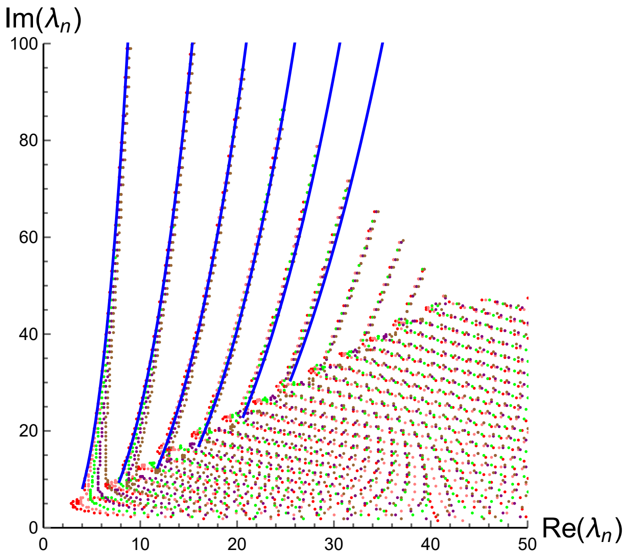

Figure 1: Trajectory in $\mathbb{C}$ of eigenvalues of truncations T_n of T_∞ from (8) for $d = 3$, $s_n = 0.1n$, $n = 15, 16, \ldots, 115$; eigenvalues for $l = 1$ (red), $l = 2$ (pink), $l = 3$ (green), $l = 4$ (purple), $l = 5$ (brown) only are plotted; see (9) and Section 4.5 for details. The numerics illustrates the spectral exactness (the clusters of eigenvalues at the ray $\mathrm{e}^{\mathrm{i}\pi/4}\mathbb{R}_+$) as well as the eigenvalues escaping to infinity along the blue curves, (9) for asymptotic formulas.

in $L^2(\Omega)$ with $\Omega = \mathbb{R}^d \setminus \overline{B_1(0)}$ and the Dirichlet boundary condition imposed at $\partial\Omega$. A possible sequence of truncations are $T_n = -\Delta_{\mathrm{D}} + Q$ in $L^2(\Omega_n)$ with $\Omega_n := B_{s_n}(0) \cap \Omega$, $s_n \nearrow +\infty$, and Dirichlet boundary conditions at $\partial\Omega_n$, $n \in \mathbb{N}$. The general goal is to determine the relation of spectra of $\{T_n\}$ and T_∞. We are able to obtain asymptotic formulae for the diverging eigenvalues, in particular in example (8), our results show that the truncations T_n contain asymptotically the diverging eigenvalues

$$\lambda_{k,n,l} = (2s_n)^{\frac{2}{3}} \left(\overline{\nu_k} + \mathcal{O}_{k,l}\left(s_n^{-\frac{4}{3}} \right) \right) + \mathrm{i}s_n^2, \quad n \to \infty, \tag{9}$$

where $\{\nu_k\}$ are eigenvalues of the imaginary Airy operator $-\partial_x^2 + \mathrm{i}x$ in $L^2(\mathbb{R}_+)$ with Dirichlet boundary condition at 0.

Concerning notation, we write $a \lesssim b$ to denote that, given $a, b \geq 0$, there exists a constant $C > 0$, independent of any relevant variable or parameter, such that $a \leq Cb$; $a \gtrsim b$ is analogous and $a \approx b$ means that $a \lesssim b$ and $a \gtrsim b$.

Chapter 1

Perturbation methods in quantum mechanics

As we already mentioned, we have to use perturbation theory and other approximative construction techniques in most cases of practical interest where usually, a key attention is being paid to Hamiltonians H.

First we recall basic notions. Let H be a closed operator $H \in C(\mathcal{H})$, then $\rho(H) := \{\lambda \in \mathbb{C} : (H-\lambda)^{-1}$ is bounded operator on $\mathcal{H}\}$ denote its resolvent set and $\sigma(H) := \mathbb{C} \setminus \rho(H)$ its spectra. The $\varepsilon-$pseudospectrum $\sigma_\varepsilon(H)$ of H is defined as [36, Chap.4]

$$\sigma_\varepsilon(H) = \sigma(H) \cup \{\lambda \in \mathbb{C} : \|(H-\lambda)^{-1}\| > \frac{1}{\varepsilon}\}, \quad \varepsilon > 0. \tag{1.1}$$

Specifically for self-adjoint operators, which will be discussed throughout this chapter, $\varepsilon-$pseudospectrum contains the spectrum $\sigma(H)$ and its $\varepsilon-$neighbourhood, since following equality holds [20, Sec.V.3.5]

$$\|(H-\lambda)^{-1}\| = \frac{1}{\operatorname{dist}(\lambda, \sigma(H))}. \tag{1.2}$$

Now, we are prepared to study the influence of perturbations.

1.1 Perturbation of potential

Alternative equivalent definition of $\varepsilon-$pseudospectra

$$\sigma_\varepsilon(H) = \{\lambda \in \mathbb{C} : \lambda \in \sigma(H+E) \text{ for some } E \in B(\mathcal{H}), \|E\| < \varepsilon\} \tag{1.3}$$

describes the stability of the spectra $\sigma(H)$ for self-adjoint operators with respect to bounded perturbation, *i.e.* the spectra $\sigma(H+E)$ of the boundedly perturbed operator $H+E$ lies in $\varepsilon-$neighbourhood of the spectra of $\sigma(H)$ of the unperturbed operator H.

Broader concept is provided by the notion of relative boundedness of forms [20, Sec. VI.1.6] or operators [30, Sec. X.2]. In such a scenario we can safely apply the Rayligh-Schrödinger perturbation theory [31, Thm. XII.8].

Quantum square well with logarithmic central spike

In [42] we introduced a linearized model of non-linear logarithmic Schrödinger equation. In particular operator $T_g = T_0 + gV$, $g \in \mathbb{R}$ such as

$$T_g = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + g \ln \frac{1}{x^2} \ , \tag{1.4}$$

acting on $L^2(\mathcal{I})$, $\mathcal{I} = (-1, 1)$, subject to Dirichlet boundary conditions.

The unperturbed operator T_0 represents the well known problem of Laplace operator on a bounded interval. Starting with a quadratic form

$$t_0[f] = \|f'\|^2 \ , \qquad D(t_0) = W_0^{1,2}(\mathcal{I}) \ , \tag{1.5}$$

it can be defined via representation theorem [20, Sec. VI.2.2] as a self-adjoint on $D(T_0) = W^{2,2}(\mathcal{I}) \cap W_0^{1,2}(\mathcal{I})$ with discrete spectrum

$$\lambda_n^{(0)} = \left[(n+1)\frac{\pi}{2}\right]^2 \ , \quad n = 0, 1, 2 \ldots, \tag{1.6}$$

and eigenfuctions

$$\psi_n^{(0)}(x) = \begin{cases} \cos(n+1)\frac{\pi}{2}x \ , & n \text{ odd} \ , \\ \sin(n+1)\frac{\pi}{2}x \ , & n \text{ even} \ . \end{cases} \tag{1.7}$$

Let

$$v[f] = \int_{\mathcal{I}} V|f|^2, \quad D(v) = \{f \in L^2(\mathcal{I}) : V|f|^2 \in L^1(\mathcal{I})\} \ , \quad V = \ln \frac{1}{x^2} \tag{1.8}$$

We note that $V \in L^p(\mathcal{I})$, $1 \le p < \infty$ since it is an even function and, for every small $\epsilon > 0$,

$$\int_0^1 \frac{x^\epsilon |\ln x|^p}{x^\epsilon} \,\mathrm{d}x \le \|x^\epsilon |\ln x|^p\|_{L^\infty} \int_0^1 x^\epsilon \,\mathrm{d}x < \infty. \tag{1.9}$$

Recalling the embedding $W^{1,2}(\mathcal{I}) \hookrightarrow L^\infty(\mathcal{I})$, *i.e.* the inequality $\|f\|_{\infty,\mathcal{I}} \le C\|f\|_{W^{1,2}}$, for some $C > 0$ and Young's inequality, we get that, for all $f \in \mathrm{Dom}(t_0)$,

$$\begin{aligned} |v[f]| &\le C\|f\|_{W^{1,2}}^2 \|V\|_{L^1} \le C\|V\|_{L^1}(2\|f'\|\|f\| + \|\eta'\|_\infty \|f\|^2) \\ &\le \delta\|f'\|^2 + +C_\delta\|f\|^2 \end{aligned} \tag{1.10}$$

where

$$C_\delta = \delta^{-1}\|V\|_{L^1}^2 + \|\eta'\|_\infty \|V\|_{L^1} \tag{1.11}$$

with $\eta \in C^\infty(\mathbb{R})$ such that

$$\eta(t) = \begin{cases} 1 & t \geq x \\ 0 & t \leq x-1 \end{cases} \tag{1.12}$$

for $x \in \mathbb{R}$ and $\delta > 0$ can be chosen arbitrarily small. Hence $D(v) \subset D(t_0)$ and v is a relatively bounded with respect to t_0 with relative bound 0. Therefore for every $g \in \mathbb{R}$, the form

$$t_g[f] = t_0[f] + gv[f], \quad D(t_g) = D(t_0) = W_0^{1,2}(\mathcal{I}) \tag{1.13}$$

is closed, symmetric and bounded from below, hence it defines (via the representation theorem) the self-adjoint operator T_g, $g \in \mathbb{R}$.

Also T_g forms an analytic family and subsequently, for g small we can compute the eigenvalues of T_g via Rayleigh-Schrödinger perturbation theory

$$\lambda_{n,g} = \lambda_n^{(0)} + g\lambda_n^{(1)} + \dots. \tag{1.14}$$

The first order corrections can be obtained in a closed form

$$\begin{aligned} \lambda_{2p}^{(1)} &= 2 + \frac{2}{(2p+1)\pi}\mathrm{Si}[(2p+1)\pi] \ , \quad p = 0,1,2\dots \\ \lambda_{2q+1}^{(1)} &= 2 - \frac{2}{(2q+2)\pi}\mathrm{Si}[(2q+2)\pi] \ , \quad q = 0,1,2\dots \end{aligned} \tag{1.15}$$

where $\mathrm{Si}(x) = \int_0^x \frac{\sin(t)}{t}\,\mathrm{d}t$ is sine-integral special function. Precision of the first order corrections for g small is demonstrated in Fig.1.1.

1.2 Asymptotic regime

Yet another definition of $\varepsilon-$pseudospectra

$$\lambda \in \sigma_\varepsilon(H) \iff \lambda \in \sigma(H) \text{ or } \exists f \in \mathrm{Dom}(H) : \|(H-\lambda)f\| < \varepsilon\|f\| \tag{1.16}$$

where f are corresponding pseudomodes, or $\varepsilon-$pseudo-eigenvectors.

Lets have a sequence of self-adjoint operators A_g acting on a sequence of Hilbert spaces $\mathcal{H}_g$. Suppose we can construct a sequence of pseudomodes $f_{n,g} \in \mathrm{Dom}(A_g)$ for some known numbers $\{\lambda_n\}$ (*i.e.* eigenvalues of a know operator A) such as

$$\|(A_g - \lambda_n)f_{n,g}\| \leq \varepsilon_g \|f_{n,g}\|, \quad \varepsilon_g > 0. \tag{1.17}$$

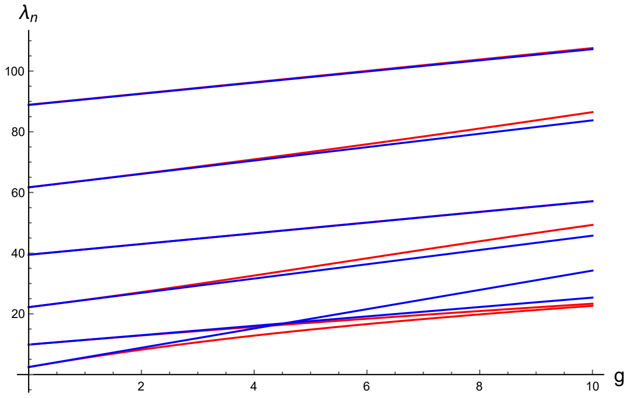

Figure 1.1: First 6 eigenvalues $\lambda_{n,g}$ of T_g 1.4 depending on g computed numerically (red) and via perturbation theory (blue) (1.14).

Latter means that $\lambda_n \in \sigma_{\varepsilon_g}(A_g)$ and therefore $\sigma(A_g) \cap [\lambda_n - \varepsilon_g, \lambda_n + \varepsilon_g] \neq \emptyset$. Furthermore if $\varepsilon_g \to 0$ as $g \to \infty$ it follows that the eigenvalues

$$\lambda_{n,g} = \lambda_n + \mathcal{O}(\varepsilon_g), \quad g \to \infty \tag{1.18}$$

are asymptotically contained in $\sigma(A_g)$.

1.2.1 Linear approximation of the potential

One specific scenario of such problems is a sequence of operators A_g

$$A_g^{(i)} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + x + R_g(x), \quad \text{in } L^2(\mathcal{I}_g) \tag{1.19}$$

where $\mathcal{I}_g \to \mathbb{R}_+$ and $R_g(x) \to 0$ as $g \to \infty$ and Dirichlet $A_g^{(1)}$ or Neumann $A_g^{(2)}$ boundary conditions are imposed on the endpoints of the interval $\mathcal{I}_g$.

In the limit, we are getting to the well know problem of Airy operator on a half-line $A_\infty^{(1)}$ (resp. $A_\infty^{(2)}$) on $L^2(0, \infty)$ with Dirichlet (resp. Neumann) boundary condition at 0

$$A_\infty^{(1)} := -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + x \ , \quad D(A_\infty) = \{W^{2,2}(\mathbb{R}_+) : f(0) = 0, xf(x) \in L^2(\mathbb{R}_+)\} \ ,$$
$$A_\infty^{(2)} := -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + x \ , \quad D(A_\infty) = \{W^{2,2}(\mathbb{R}_+) : f'(0) = 0, xf(x) \in L^2(\mathbb{R}_+)\} \ .$$

which possess purely discrete positive spectrum

$$\sigma(A_\infty^{(i)}) = \{\lambda_n^{(i)}\}, \quad \lambda_n^{(1)} = -a_n, \quad \lambda_n^{(2)} = -b_n \tag{1.20}$$

where a_n satisfy $\mathrm{Ai}(a_n) = 0$ and b_n satisfy $\mathrm{Ai}'(b_n) = 0$ for the Airy function

$$\mathrm{Ai}(x) = \frac{1}{\pi} \int_0^\infty \cos\left(\frac{t^3}{3} + xt\right) \mathrm{d}t \; . \tag{1.21}$$

Corresponding eigenfunctions of $A_\infty^{(i)}$ are shifted Airy functions

$$\psi_n^{(i)}(x) = \mathrm{Ai}(x - \lambda_n^{(i)}). \tag{1.22}$$

In such a setting, if for some sequence of pseudomodes $f_{n,g}^{(i)} \in \mathrm{Dom}(A_g^{(i)})$ it holds that

$$\|(A_g^{(i)} - \lambda_n^{(i)}) f_{n,g}^{(i)}\| \leq \varepsilon_g^{(i)} \|f_{n,g}^{(i)}\| \tag{1.23}$$

such that $\varepsilon_g^{(i)} \to 0$ as $g \to \infty$, we get that

$$\lambda_{n,g}^{(i)} = \lambda_n^{(i)} + \mathcal{O}(\varepsilon_g^{(i)}), \quad g \to \infty \tag{1.24}$$

lie asymptotically in the spectra of $A_g^{(i)}$.

Quantum square well with logarithmic central spike

The Example 1.1 can be investigated also in the setting of strong coupling $g \gg 1$. In such a scenario the spectrum of T_g (1.4) is shifted upwards. We claim that the spectrum of T_g asymptotically contains the eigenvalues

$$\lambda_n(g) = \begin{cases} -(2g)^{2/3}(a_n + \mathcal{O}(g^{-\frac{4}{3}+\varepsilon})) \; , & \text{odd } n \; , \\ -(2g)^{2/3}(b_n + \mathcal{O}(g^{-\frac{4}{3}+\varepsilon})) \; , & \text{even } n \; . \end{cases} \tag{1.25}$$

The potential $V(x,g) = g \ln(\frac{1}{x^2})$ is even therefore the eigenfunctions of T_g are even or odd and we can split the problem into two cases

$$T_g^{(1)} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + g \ln\frac{1}{x^2} \text{ acting on } L^2(0,1) \text{ with } \psi(0) = 0, \psi(1) = 0 \tag{1.26}$$

$$T_g^{(2)} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + g \ln\frac{1}{x^2} \text{ acting on } L^2(0,1) \text{ with } \psi'(0) = 0, \psi(1) = 0 \tag{1.27}$$

The spectrum of the operator T_g is than obtained as a union of respective spectra

$$\sigma(T_g) = \sigma(T_g^{(1)}) \cup \sigma(T_g^{(2)}). \tag{1.28}$$

Unitary transformations $\mathcal{P} : L^2(0,1) \mapsto L^2(0,1)$ such that $(\mathcal{P}f)(x) = f(1-x)$ and $U_\alpha : L^2(0,1) \mapsto L^2(0,\sigma^{-1})$ such that $(U_\alpha f)(x) = \sigma^{-\frac{1}{2}} f(\sigma x)$ lead us to isospectral operators

$$\tilde{T}_g^{(i)} = \sigma^{-2} A_g = \sigma^{-2} \left[-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \sigma^2 g \ln\frac{1}{(1-\sigma x)^2} \right] \tag{1.29}$$

acting on $L^2((0,\sigma^{-1}))$. Employing further Taylor expansion of logarithmic term and choosing $\sigma = (2g)^{-\frac{1}{3}}$ in order to get the linear term dominant we get

$$A_g^{(i)} = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + x + \sigma^2 R_1(\sigma x, g), \quad L^2((0,(2g)^{\frac{1}{3}})). \tag{1.30}$$

We can see that (1.30) is in the form (1.19) and in order to prove validity of the asymptotic formula (1.24) we need to show that for some $f_{n,g} \in \mathrm{Dom}(A_g)$

$$\|(A_g^{(i)} - \lambda_n^{(i)})f_{n,g}^{(i)}\| \leq \varepsilon_g^{(i)} \|f_{n,g}^{(i)}\| \tag{1.31}$$

such that $\varepsilon_g^{(i)} \to 0$ as $g \to \infty$.

Let $f_{n,g}^{(i)} = \psi_n^{(i)} \phi_g$ where $\psi_n^{(i)}$ are eigenfunctions of Airy operators (1.22), $\phi_g = \phi(((2g)^{\frac{1}{3}})^{-\beta} x)$, $\beta \in (0,1)$ and $\phi \in C^\infty(\mathbb{R}_+)$ such that

$$\phi(x) = \begin{cases} 1 & x \in [0,1/2] \\ 0 & x \geq 1 \end{cases} \tag{1.32}$$

We can estimate

$$\begin{aligned} \|(A_g^{(i)} - \lambda_n^{(i)})f_{n,g}^{(i)}\| \leq \|(-\psi_n^{(i)\prime\prime} + x\psi_n^{(i)} - \lambda_n^{(i)}\psi_n^{(i)})\phi_g\| + \|\psi_n^{(i)\prime}\phi_g'\| \\ + \|\psi_n^{(i)}\phi_g''\| + \|\sigma^2 R_1(\sigma x, g)\psi_n^{(i)}\phi_g\|. \end{aligned} \tag{1.33}$$

The first term is equal to 0 since $\psi_n^{(i)}, \lambda_n^{(i)}$ are eigenfunctions and eigenvalues of the Airy operators. For second and third term we use the knowledge of the asymptotic behaviour of the Airy function

$$\|\psi_n^{(i)\prime}\phi_g'\|^2 \leq (2g)^{-\frac{\beta}{3}} \int_{(2g)^{\frac{\beta}{3}}/2}^{(2g)^{\frac{\beta}{3}}} |\psi_n^{(i)\prime}|^2 \lesssim \mathrm{e}^{-(2g)^\beta} \tag{1.34}$$

since $\mathrm{Ai}(x) \lesssim \mathrm{e}^{-x^{\frac{3}{2}}}$ and $\mathrm{Ai}'(x) \lesssim \mathrm{e}^{-x^{\frac{3}{2}}}$ [28, p. 394]

$$\|\psi_n^{(i)}\phi_g''\|^2 \leq (2g)^{-\frac{2\beta}{3}} \int_{(2g)^{\frac{\beta}{3}}/2}^{(2g)^{\frac{\beta}{3}}} |\psi_n^{(i)}|^2 \lesssim (2g)^{-\frac{\beta}{3}} \mathrm{e}^{-(2g)^\beta}. \tag{1.35}$$

For the last term we use the Lagrange form of the remainder with $\xi \in [0,x]$

$$\begin{aligned} &\|\sigma^2 R_1(\sigma x)\psi_n^{(i)}\phi_g(x)\|^2 \leq \sigma^4 \int_0^{(2g)^{\frac{\beta}{3}}} |R_1(\sigma x)|^2 |\psi_n^{(i)}(x)|^2 \mathrm{d}x \\ &\leq 3(2g)^{-\frac{8}{3}} \int_0^{(2g)^{\frac{\beta}{3}}} |(1-(2g)^{-\frac{1}{3}}\xi)^2 x^2|^2 |\psi_n^{(i)}(x)|^2 \mathrm{d}x \\ &\lesssim (2g)^{\frac{4\beta-8}{3}} \|\psi_n^{(i)}\|_{L^2(\mathbb{R}_+)} \sim g^{-\frac{8}{3}+\frac{4\beta}{3}}, \quad g \to \infty \end{aligned} \tag{1.36}$$

with the choice $\beta = 3/2\varepsilon$. (1.31) therefore holds with $\varepsilon_g = g^{-\frac{4}{3}+\varepsilon}$ and (1.25)

1.2.2 Quadratic approximation of the potential

Another scenario widely used in physics is approximation of Schrödinger operator whose potential posses profound minimum by quantum harmonic oscillator. Eligible sequence of operators would after suitable transformation have a form

$$A_g = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + x^2 + R(x,g), \quad L^2(\mathcal{I}_g), \tag{1.37}$$

where $R(x,g) \to 0$ and $\mathcal{I}_g \to \mathbb{R}$ as $g \to \infty$. Solving a problem we usually encounter operator

$$H_g = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + W(x,g), \quad \text{ in } L^2(\mathcal{J}_g) \tag{1.38}$$

where potential $W(x,g)$ posses minimum at some point x_0 such as

$$W(x_0,g) = 0, \quad W'(x_0,g) = 0, \quad W''(x_0,g) > 0 \tag{1.39}$$

Translation to x_0, subtracting and absolute term $W(x_0,g)$

$$T_g = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + W(x+x_0,g) - W(x_0,g), \quad L^2(\mathcal{J}_g - (x_0,x_0)) \tag{1.40}$$

and further expanding the Taylor series about 0 and scaling $x \to \sigma x$,

$$\sigma = \left(\frac{1}{2}\frac{\mathrm{d}^2 W(x+x_0,g)}{\mathrm{d}x^2}\Big|_{x=0}\right)^{-\frac{1}{4}} \tag{1.41}$$

in order to make factor in front of the quadratic term equal to 1. We arrive at a form

$$\sigma^{-2} A_g = \sigma^{-2}\left[-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + x^2 + \sigma^2 R_2(\sigma x, g)\right]. \tag{1.42}$$

From transformations above, we get that

$$\lambda_{n,g} \in \sigma(A_g) \iff \sigma^{-2}\lambda_{n,g} + W(x_0,g) \in \sigma(H_g). \tag{1.43}$$

Formula for the eigenvalues $\lambda_{n,g} \in \sigma(A_g)$ can be obtained in similar manner as for the linear approximation using eigenvalues $\lambda_n = 2n+1$ and eigenfunctions $h_n(x)$ of one-dimensional quantum harmonic oscillator

$$A = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + x^2, \quad L^2(\mathbb{R}) \tag{1.44}$$

where $h_n(x)$ are normed Hermite functions.

If we are able to construct sequence of pseudomodes $f_{n,g} \in \mathrm{Dom}(A_g)$ such that

$$\|(A_g - \lambda_n) f_{n,g}\| \leq \varepsilon_g \|f_{n,g}\| \tag{1.45}$$

and $\varepsilon_g \to 0$. Then the eigenvalues

$$\lambda_{n,g} = 2n + 1 + \mathcal{O}(\varepsilon_g), \quad g \to \infty \tag{1.46}$$

lie asymptotically in the spectra of A_g.

Log-anharmonic oscillator

In [41] we derived following log-anharmonic model

$$H_g = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \omega^2 x^2 + g^2 \ln \frac{1}{x^2} \quad \text{in } L^2(\mathbb{R}). \tag{1.47}$$

In what follows, we prove that there are asymptotically contained double degenerate eigenvalues

$$\lambda_{n,g} = \sqrt{2}\omega((2n+1) + \mathcal{O}(g^{-1+\epsilon})) + g^2 + g^2 \ln \frac{\omega^2}{g^2}, \quad g \to \infty \tag{1.48}$$

in the spectra of H_g.

Unitary operation of translation to the minimum $x_0 = \frac{g}{\omega}$ and subsequent subtraction of the absolute term $g^2 + g^2 \ln \frac{\omega^2}{g^2}$ get us to

$$T_g = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + \omega^2 x^2 + 2\omega g x + g^2 \ln \frac{1}{(x + g/\omega)^2} - g^2 \ln \frac{\omega^2}{g^2} \tag{1.49}$$

acting in $L^2(\mathbb{R})$. Further expanding to Taylor series and scaling with $\sigma = (2\omega^2)^{-\frac{1}{4}}$ we get

$$\sqrt{2}\omega \left[-\frac{\mathrm{d}^2}{\mathrm{d}x^2} + x^2 + (\sqrt{2}\omega)^{-1} R_2(\sigma x) \right], \tag{1.50}$$

which corresponds with (1.42). In order to prove the asymptotic formula (1.43), we need to construct sequence of pseudomodes $f_{n,g}$. Let

$$f_{n,g}(x) := h_n(x) \varphi_g(x), \tag{1.51}$$

where $h_n(x)$ are normed Hermite functions and $\varphi_g(x) = \varphi(g^{-\beta} x)$, $\beta > 0$ and $\varphi \in C_0^\infty(\mathbb{R})$ such that

$$\varphi(x) = \begin{cases} 1 & |x| \leq 1, \\ 0 & |x| \geq 2. \end{cases} \tag{1.52}$$

It follows that $\varphi_g(x) = 0$ for $|x| \geq 2g^\beta$ and $\|f_{n,g}\|_{L^2(\mathbb{R})} \to 1$ as $g \to \infty$. Now, we can estimate

$$\begin{aligned} \|(A_g - \lambda_n) f_{n,g}\| \leq & \|(-h_n'' + x^2 h_n - \lambda_n h_n)\varphi_g\| + \|2h_n'\varphi_g'\| \\ & + \|h_n \varphi_g''\| + \|\sigma^2 R_2(\sigma x, g) h_n \varphi_g\|, \end{aligned} \tag{1.53}$$

The first term is equal to zero since h_n and λ_n are eigenfuctions and eigenvalues of A (1.44). We will estimate the remaining terms via the knowledge of the behaviour of the Hermite functions.

$$\begin{aligned} \|2h_n'\varphi_g'\|^2 &\leq 4g^{-2\beta} \int_{\mathbb{R}} |h_n'(x)|^2 |\varphi'(g^{-\beta}x)|^2 \mathrm{d}x \\ &\leq 8g^{-2\beta} \int_{g^\beta}^{2g^\beta} |h_n'(x)|^2 \mathrm{d}x \lesssim g^{-\beta} \mathrm{e}^{-\tilde{\delta}_n g^{2\beta}} \end{aligned} \tag{1.54}$$

since $|h_n'(x)| \leq \mathrm{e}^{-\delta_n x^2}$. Similarly

$$\|h_n \varphi_g''\|^2 \leq 2g^{-4\beta} \int_{g^\beta}^{2g^\beta} |h_n(x)|^2 \mathrm{d}x \lesssim g^{-3\beta} \mathrm{e}^{-\delta_n g^{2\beta}}. \tag{1.55}$$

To estimate the last term we use the Lagrange form of the remainder and scaling $\sigma x = y$, for any constant $\omega \in \mathbb{R}$ we have

$$\begin{aligned} & \|\sigma^2 R_2(\sigma x, g) h_n \varphi_g\|^2 \\ & \leq \sigma^3/36 \int_{\mathbb{R}} |W'''(\xi, g)|^2 |y|^6 |h_n(\sigma^{-1}y)|^2 |\varphi(g^{-\beta}\sigma^{-1}y)|^2 \mathrm{d}y \\ & \leq \sigma^3/36 \; (2\sigma g^\beta)^6 \sup_{|\xi| \leq |2\sigma g^\beta} ||W'''(\xi, g)|^2 \int_{|y| \leq 2\sigma g^\beta} |h_n(\sigma^{-1}y)|^2 \mathrm{d}y \\ & \lesssim \sigma^{10} g^{6\beta} \sup_{|\xi| \leq |2\sigma g^\beta|} \left| \frac{4g^2}{(x + g/\omega)^3} \right|^2 \lesssim \frac{g^{4+6\beta}}{g/\omega - 2g^\beta \sigma} \sim g^{-2+6\beta}, \quad g \to \infty \end{aligned} \tag{1.56}$$

with the choice $\beta = \varepsilon/3$, $\varepsilon > 0$ we get

$$\frac{\|(A_g - \lambda_n) f_{n,g}\|}{\|f_{n,g}\|} \lesssim g^{-1+\varepsilon}. \tag{1.57}$$

Finally we obtain (1.48) from (1.43).

Similarly we can perform a translation to $-x_0 = -g/\omega$, proceeding with analogous steps we obtain second set of the same eigenvalues $\lambda_{n,g}$. Therefore the eigenvalues (1.48) are double-degenerate.

method:	n=0	n=1	n=2	n=3	n=4
quadratic approx.	0.00141421	0.00424264	0.00707107	0.00989949	0.0127279
numerical	0.00141432	0.00424309	0.00707218	0.00990161	0.0127314

Table 1.1: A sample of the low-lying energy-level shifts $\epsilon_{n,g} = \lambda_{n,g} - g^2 - g^2 \ln \frac{\omega^2}{g^2}$ for couplings $\omega = 0.001$ and $g = 1$.

Singular model

In article [5] we considered a model

$$H_g = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + x + \frac{2g}{\sqrt{x}}, \qquad \text{in } L^2(\mathbb{R}_+), \tag{1.58}$$

where we can impose Dirichlet or Neumann boundary conditions at the origin. In the asymptotic scenario $g \to \infty$ specific boundary conditions do not play significant role. We will prove that the eigenvalues

$$\lambda_{n,g} = \frac{\sqrt{3}}{2} g^{-\frac{1}{3}}((2n+1) + \mathcal{O}(g^{-\frac{1}{2}+\varepsilon})) + 3g^{\frac{2}{3}}, \quad g \to \infty. \tag{1.59}$$

are asymptotically contained in $\sigma(H_g)$.

Similarly as above, we perform translation to the minimum $x_0 = g^{\frac{2}{3}}$ and subtraction of the absolute term $W(x_0, g) = 3g^{\frac{2}{3}}$ we get

$$T_g = -\frac{\mathrm{d}^2}{\mathrm{d}x^2} + x + \frac{2g}{\sqrt{x + g^{\frac{2}{3}}}} - 2g^{\frac{2}{3}}, \qquad \text{in } L^2((-g^{\frac{2}{3}}, \infty)) \tag{1.60}$$

Scaling with $\sigma = (\frac{3}{4})^{-\frac{1}{4}} g^{\frac{1}{6}}$ yields the required result. Construction of $f_{n,g}$ proceeds in similar manner

$$f_{n,g}(x) := \chi_{\mathcal{I}_g} h_n(x) \varphi_g(x), \tag{1.61}$$

where $h_n(x)$ are normed Hermite functions, $\mathcal{I}_g = (-g^{\frac{2}{3}}, \infty)$ and $\varphi_g(x) = \varphi(\sigma^{-\beta} x)$, $\beta > 0$ and $\varphi \in C_0^\infty(\mathbb{R})$ is as in (1.52). The estimates (1.54),(1.55) are done in analogous manner. Concerning the term with the remainder employing scaling $\sigma x = y$ we have

$$
\begin{aligned}
&\|\sigma^2 R_2(\sigma x, g) h_n \varphi_g\|^2 \\
&\leq \sigma^3/36\ (2\sigma\sigma^\beta)^6 \sup_{|\xi|\leq|2\sigma\sigma^\beta} ||W'''(\xi,g)|^2 \int_{|y|\leq 2\sigma\sigma^\beta} |h_n(\sigma^{-1}y)|^2 \mathrm{d}y \\
&\lesssim \sup_{|\xi|\leq|2(\frac{3}{4})^{-\frac{1}{4}} g^{\frac{\beta+1}{6}}|} \left| \frac{g}{(x+g^{\frac{2}{3}})^{\frac{7}{2}}} \right|^2 \left(\frac{3}{4}\right)^{-\frac{1}{4}} g^{\beta+\frac{5}{3}} \\
&\lesssim \frac{g^{\beta+\frac{11}{3}}}{|g^{\frac{2}{3}} - c g^{\frac{\beta+1}{6}}|^7} \sim g^{-1+\beta} \to 0, \quad g \to \infty
\end{aligned}
\tag{1.62}
$$

with the choice $\beta = 2\varepsilon$, $\varepsilon > 0$. Altogether we arrive at our result (1.59). In table 1.2 we can see, that the error of the perturbative approach in comparison with the numerical solution is of order 10^{-7} to 10^{-5}.

method:	n=0	n=1	n=2	n=3	n=4
quadratic approx.	0.0401978	0.120592	0.200985	0.281381	0.361778
numerical	0.0401977	0.120590	0.200981	0.281370	0.361757

Table 1.2: A sample of the low-lying energy-level shifts $\epsilon_{n,g} = \lambda_{n,g} - 3g^{\frac{2}{3}}$ for coupling $g = 10000$.

Chapter 2

Quasi-self-adjoint quantum observables

Special subclass of non-self-adjoint operators is presented by *quasi-self-adjoint operators*. First discussed in [16] and later introduced in nuclear physics paper [33], quasi-self-adjoint operators satisfy

$$H^* = \Theta H \Theta^{-1} \tag{2.1}$$

for some positive, bounded and boundedly invertible operator Θ called *metric*. We can introduce new inner product in the underlying Hilbert space

$$\langle \cdot, \cdot \rangle_\Theta = \langle \cdot, \Theta \cdot \rangle \tag{2.2}$$

quasi-self-adjoint operator H can be defined as self-adjoint with respect to the new inner product (2.2). Moreover, H is quasi-self-adjoint if and only if it is similar to a self-adjoint operator h, *i.e.*

$$h = \Omega H \Omega^{-1} \tag{2.3}$$

where Ω is bounded and boundedly invertible operator. (2.1) follows from (2.3) with special choice $\Theta := \Omega^* \Omega$, also (2.3) follows from (2.1) with special choice $\Omega := \Theta^{\frac{1}{2}}$.

This can be put into a framework of three Hilbert spaces, *i.e.*H is quasi-self-adjoint operator in the first Hilbert space with standard inner product, H is self-adjoint operator in the second space with modified inner product (2.2) and h is self-adjoint operator in the third Hilbert space, which may in general have different underlying vector space. For further details on three-Hilbert-space formulation of quantum mechanic see [40].

It follows from (2.3) that the spectra of quasi-self-adjoint operator is purely real. For pseudospectra of a similar operator it holds that

$$\sigma_{\varepsilon/\kappa}(H) \subseteq \sigma_\varepsilon(h) \subseteq \sigma_{\varepsilon\kappa} \tag{2.4}$$

where $\kappa := \|\Omega\|\|\Omega^{-1}\|$. For quasi-self-adjoint operators κ is finite and therefore for their pseudospectra we have that

$$\sigma_\varepsilon(H) \subset \{z \in \mathbb{C} : \mathrm{dist}(z, \sigma(H)) < \kappa\varepsilon\}. \tag{2.5}$$

2.1 Construction of metric operator

Eigenvectors $\{\psi_n\}_n$ of quasi-self-adjoint operator H with compact resolvent form a *Riesz basis*, *i.e.* a basis that can be mapped via bounded and boundedly invertible linear operator to an orthonormal basis. Equivalently, if it forms a basis and there exists $C > 0$ such that

$$\forall \psi \in \mathcal{H}, \quad C^{-1}\|\psi\|^2 \leq \sum_{k=1}^{\infty} |\langle \psi_k, \psi \rangle|^2 \leq C\|\psi\|^2. \tag{2.6}$$

Eigenfunctions of an operator with compact resolvent and purely real eigenvalues form a Riesz basis if and only if the operator is quasi-self-adjoint [21, Prop. 1.5.4]. Together with the eigenfuctions $\{\phi_n\}_n$ of the adjoint operator H^* they form a complete biorthonormal system

$$(\psi_m, \phi_n) = \delta_{mn}, \quad \sum_n \psi_n(\phi_n, \cdot) = I. \tag{2.7}$$

For a diagonalizable operator H we have following spectral representation

$$H = \sum_n \lambda_n \psi_n(\phi_n, \cdot) \ , \quad H^* = \sum_n \lambda_n \phi_n(\psi_n, \cdot) \ . \tag{2.8}$$

and the metric operator Θ may be computed as

$$\Theta = \sum_n \kappa_n \phi_n(\phi_n, \cdot), \tag{2.9}$$

where κ_n are positive and properly bounded $C^{-1} \leq \kappa_n \leq C$, with some $C > 0$. Due care must be paid to the convergence of the series in the infinite-dimensional cases.

2.2 Compatibility of several quasi-Hermitian observables

In what follows, we restrict ourselves to a finite-dimensional scenario. Let $j \in \{1, 2, \ldots, p\}$, then for every quasi-self-adjoint operator $A_j \in \mathbb{C}^{N\times N}$ exists a family of admissible metrics

$$A_j^* \Theta_j = \Theta_j A_j \ , \quad \Theta_j = \sum_n^N \kappa_n^{(j)} \phi_n(\phi_n, \cdot), = \Theta(\vec{\kappa}(j)). \tag{2.10}$$

If we intend to define consistent quantum mechanical picture including all above-mentioned operators, all of them must be quasi-self-adjoint with respect to the same metric

$$\Theta_1(\vec{\kappa}^{(1)}) = \Theta_2(\vec{\kappa}^{(2)}) = \cdots = \Theta_p(\vec{\kappa}^{(p)}) \ . \tag{2.11}$$

There are three possible types of solution for the set of equation 2.11. The first, most trivial case is when the equations don't impose any conditions on the parameters $\vec{\kappa}^{(j)}$. In such a case the operators commute and eigenbasis of all the observables coincides.

If the operators don't commute, the system of equations 2.11 restricts the number of free parameters $\vec{\kappa}^{(j)}$. In special case, all the parameters are uniquely defined and we arrive at an ideal scenario presented in [33], where there is just one common metric.

The case of interest for us is the third case of nonexistence of any solution of the system of equations 2.11, *i.e.* nonexistence of a common metric for given observables. This danger is often forgotten in the literature. In the following examples, we will demonstrate, that even in finite dimension the possibility of nonexistence of a common metric cannot be ignored.

Example 2.2.1. Let $A, B \in \mathbb{C}^{N\times N}$ be our desirable quasi-self-adjoint observables with metrics $\Theta^{(A)} = \Theta^{(A)}(\vec{\alpha})$ and $\Theta^{(B)} = \Theta^{(B)}(\vec{\beta})$ respectively. From the requirements 2.11 we obtain $N(N-1)/2$ independent conditions

$$\left[U(\vec{\alpha})\, \Theta^{(B)}(\vec{\beta}(\vec{\alpha}))U^\dagger(\vec{\alpha})\right]_{mn} = 0 \ ,$$

where $U(\vec{\alpha})$ are unitary matrices diagonalizing $\Theta^{(A)}(\vec{\alpha})$ and $m = n+1, n+2, \ldots, N, \quad n = 1, 2, \ldots, N-1$.

N parameters of $\vec{\alpha}$ are constrained by the set of the $N(N-1)/2$ complex nonlinear, therefore we have $N(N-1)$ real algebraic equations. For $N > 2$ the nontrivial real and positive roots α_n need not to exist at all and the common observability is not guaranteed. The case of $N = 2$ was illustrated in [27].

2.3 Small non-Hermitian perturbation

Another way how to approach the common observability problem is to assume the existence of the metric in advance and look for the conditions imposed upon the observables. *e.g.* in standard quantum mechanics, special choice of $\Theta = I$ is fixed in advance. We consider two observables $A, B \in \mathbb{C}^{N\times N}$ with small non-Hermitian perturbation (only first order correction are considered)

$$A = A_0 + \varepsilon A_1 + \dots, \quad A_0 = A_0^*, \tag{2.12}$$

$$B = B_0 + \varepsilon B_1 + \dots, \quad B_0 = B_0^*. \tag{2.13}$$

We assume existence of a metric in a form

$$\Theta = I + \varepsilon F + \dots\ , \quad F = F^* \tag{2.14}$$

and search for the conditions imposed upon the pair of perturbations A_1, B_1, or more specifically on the Hermitian matrices R, S obtained via 2.1

$$A_1 - A_1^* = iR\ , \quad R = R^*\ , \quad B_1 - B_1^* = iS\ , \quad S = S^*\ . \tag{2.15}$$

Applying properties of symmetric and antisymmetric matrices on equations 2.1 and 2.15 we arrive to N^2 real and linear equations for every observable

$$\mathcal{A}\vec{f} = \mathrm{i}\vec{r}\ , \quad \mathcal{B}\vec{f} = \mathrm{i}\vec{s}\ , \tag{2.16}$$

for which we assume the existence of common solution $\vec{f}$ (i.e. the matrix F), restricting the input parameters of the observables A, B presented in $N \times N$ matrices $\mathcal{A}, \mathcal{B}$ and vectors $\vec{r}$, $\vec{s}$.

Example 2.3.1. In the case of $N = 2$, the observables A, B and the metric operator Θ have a simple form

$$F = \begin{pmatrix} x & z+p \\ z-p & y \end{pmatrix}\ , \quad A_0 = \begin{pmatrix} a & c+d \\ c-d & b \end{pmatrix}\ , \quad R = \begin{pmatrix} r_1^{(3)} & r_2^{(3)} + r_1^{(1)} \\ r_2^{(3)} - r_1^{(1)} & r_3^{(3)} \end{pmatrix}\ ,$$

$$B_0 = \begin{pmatrix} \tilde{a} & \tilde{c}+\tilde{d} \\ \tilde{c}-\tilde{d} & \tilde{b} \end{pmatrix}\ , \quad S = \begin{pmatrix} s_1^{(3)} & s_2^{(3)} + s_1^{(1)} \\ s_2^{(3)} - s_1^{(1)} & s_3^{(3)} \end{pmatrix}\ .$$

Solving the equations 2.16, we obtain three conditions on A and B for the nontrivial common metric to exist

$$\hat{r}_2^{(3)}/d = \hat{r}_1^{(1)}/c = \hat{s}_2^{(3)}/\tilde{d} = \hat{s}_1^{(1)}/\tilde{c}\ , \tag{2.17}$$

with

$$\hat{r}_2^{(3)} = r_2^{(3)} + (b-a)p \ , \quad \hat{r}_1^{(1)} = r_1^{(1)} + (b-a)z \ ,$$
$$\hat{s}_2^{(3)} = s_2^{(3)} + (\tilde{b}-\tilde{a})p \ , \quad \hat{s}_1^{(1)} = s_1^{(1)} + (\tilde{b}-\tilde{a})z \ ,$$

where

$$z = \frac{cs_1^{(3)} - \tilde{c}r_1^{(3)}}{2(c\tilde{d} - d\tilde{c})}, \quad p = \frac{ds_1^{(3)} - \tilde{d}r_1^{(3)}}{2(c\tilde{d} - d\tilde{c})}.$$

Therefore even in the simple case of $N = 2$ existence of common metric is not guaranteed and we have to take into account the conditions (2.17) imposed upon the observables A and B.

Chapter 3

Spectra of non-self-adjoint operators

Another interesting subclass of non-self-adjoint Schrödinger operators

$$H = -\Delta + Q(x), \quad L^2(\mathbb{R}^d) \tag{3.1}$$

where $Q : \mathbb{R}^d \to \mathbb{C}$, are $\mathcal{PT}$-symmetric operators, satisfying

$$[H, \mathcal{PT}] = 0 \tag{3.2}$$

with $(\mathcal{P}\psi)(x) := \psi(-x)$ is the linear parity operator and $(\mathcal{T}\psi)(x) := \overline{\psi(x)}$ is the antilinear time-reversal operator. Their study was initiated in [8], where it was demonstrated that 1-dimensional Schrödinger operators with imaginary polynomial potentials with odd power greater than 3 posses real spectrum.

Even though many $\mathcal{PT}$-symmetric operators posses real spectra and some of them are even quasi-self-adjoint *cf.* Chap. 2, it is not true in general. $\mathcal{PT}$-symmetric operators often have complex spectra. Concerning the criteria for the reality of the spectrum and $\mathcal{PT}$-symmetric phase transition see *e.g.* [13].

Applicability of models with complex spectra was found in open systems, particularly modeling balance between gain and loss in optics [10], or the injection and removal of particles in Bose-Einstein condensates [14]. In the context of enhanced dissipation [17, 32] we encounter operators with a strongly coupled $\operatorname{Im} Q$ such as

$$T_g = -\partial_x^2 + x^2 + \mathrm{i}g(1 + |x|^\kappa)^{-1}, \tag{3.3}$$

with $\kappa, g > 0$, which are known to satisfy $\operatorname{Re}\sigma(T_g) \geq C_\kappa\, g^{\frac{2}{\kappa+2}}$ for $g > 0$, see [32]. Our results show that this bound is exhausted as $g \to +\infty$ since the spectra of T_g contain asymptotically the eigenvalues

$$\lambda_{k,g} = g^{\frac{2}{\kappa+2}}(\overline{\nu}_{k,\kappa} + o_k(1)) + \mathrm{i}g, \quad g \to +\infty, \tag{3.4}$$

where $\{\nu_{k,\kappa}\}$ are eigenvalues of $-\partial_x^2 + \mathrm{i}|x|^\kappa$ in $L^2(\mathbb{R})$, see also Figure 3.1.

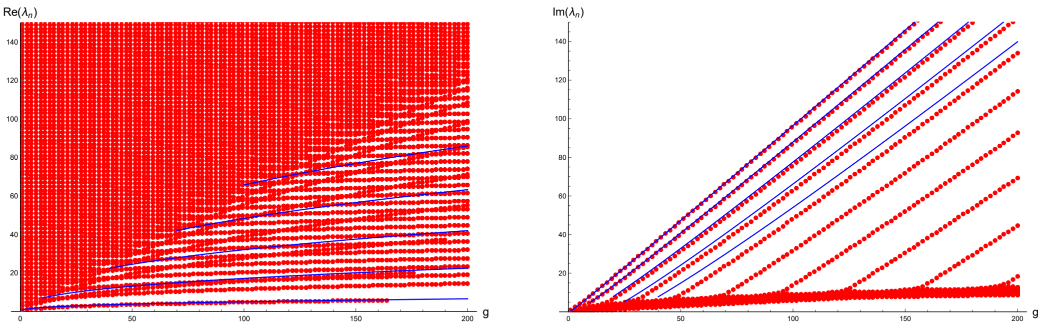

Figure 3.1: $Q_1(x) = x^2$, $Q_2(x) = (1 + |x|^\kappa)^{-1}$: Real (left) and imaginary (right) part of the eigenvalues (red) of operators T_g with $\kappa = 3.15$ and $g = 5, 10, \ldots, 200$. Asymptotic curves (blue) for $\lambda_{k,g}$ for $k = 1, 2, \ldots, 5$.

Gradually [39] the study of the spectra of non-self-adjoint operators and the behaviour of complex energies had to proceed to greater depth [4]. The former is significantly more challenging than in the case of self-adjoint operators. We cannot use the ideas of Section 1.2, since (1.2) does not hold. Instead we have following resolvent estimate [21, Prop. 1.2.3]

$$\|(H - \lambda)^{-1}\| \leq \frac{1}{\operatorname{dist}(\lambda, \overline{\operatorname{Num}(H)})} \tag{3.5}$$

where $\operatorname{Num}(H)$ is the numerical range

$$\operatorname{Num}(H) = \{(\psi, H\psi) : \psi \in \operatorname{Dom}(H), \|\psi\| = 1\} \tag{3.6}$$

H closed operator such that each connected component of $\mathbb{C} \setminus \overline{\operatorname{Num}(H)})$ has a non-empty intersection with $\rho(H)$.

Subsequently the $\varepsilon-$pseudospectrum consists not only of the spectrum $\sigma(H)$ and its $\varepsilon-$neighbourhood, but can contain also values very far from the spectra as well. The definition (1.3) now describes also the possible instability of the spectra under small bounded perturbation. In principle even the slightest perturbation can create wild changes in the spectra.

In general, spectra of non-self-adjoint operator may consist of whole complex plane or be even empty. Therefore we need to develop much more sophisticated tools including estimates for the difference of resolvents in norm and criteria for the norm resolvent convergence of a sequence of non-self-adjoint operators.

3.1 Schrödinger operators with complex potentials

Further we will discuss Schrödinger operators with complex potentials, satisfying following assumption

Assumption 3.1.1. [34, Asm. 2.1] Let $\emptyset \neq \Omega \subset \mathbb{R}^d$ be open and let $Q \in W^{1,\infty}_{\mathrm{loc}}(\overline{\Omega};\mathbb{C})$ with $\operatorname{Re} Q \geq 0$ satisfy

$$\exists \varepsilon_\nabla \in [0, \varepsilon_{\mathrm{crit}}), \quad \exists M_\nabla \geq 0, \quad |\nabla Q| \leq \varepsilon_\nabla |Q|^{\frac{3}{2}} + M_\nabla \quad \text{a.e. in } \Omega; \tag{3.7}$$

here $\varepsilon_{\mathrm{crit}} = 2 - \sqrt{2}$. ■

The Dirichlet realization T of $-\Delta + Q$ in $L^2(\Omega)$ can be obtained via the form

$$t[f] := \|\nabla f\|^2 + \int_\Omega Q(x)|f(x)|^2 \,\mathrm{d}x, \quad \mathrm{Dom}(t) := W^{1,2}_0(\Omega) \cap \mathrm{Dom}(|Q|^{\frac{1}{2}}) \tag{3.8}$$

invoking the generalization of Lax-Milgram theorem [2]. The associated operator is defined in the usual way

$$\begin{aligned} \mathrm{Dom}(T) &:= \{f \in \mathrm{Dom}(t) \,:\, \exists \eta \in L^2(\Omega),\ \forall g \in \mathrm{Dom}(t),\ t(f,g) = \langle \eta, g\rangle\}, \\ Tf &:= \eta = -\Delta f + Qf. \end{aligned} \tag{3.9}$$

Operator T is m-accretive, further known properties of such operators are summarized in [34, Thm. 2.2] based on previous works [2, 22].

3.2 Perturbation in domain and potential

For $j = 1, 2$, we consider the Dirichlet realizations

$$T_j = -\Delta + Q_j, \quad L^2(\Omega_j) \tag{3.10}$$

with open $\Omega_j \subset \mathbb{R}^d$ introduced in the same manner as in Section 3.1. In order to learn any information about the distance of their spectra, we need to study the difference of their resolvents in norm $\|R_1(z) - R_2)(z)\|$, where $R_j(z) := (T_j - z)^{-1}$, $j = 1, 2$ for $z \in \rho(T_j)$.

Further we discuss not only perturbation in the potential but also perturbation in the domain. Let us assume that following assumption on the domains holds

Assumption 3.2.1. [34, Asm. 3.1] Let $\Omega_0 := \Omega_1 \cup \Omega_2$ and suppose that Ω_1 and Ω_2 are such that there exists a cut-off $\xi : \Omega_0 \to [0,1]$ satisfying that $\chi_{\Omega_1 \cap \Omega_2}\xi = \xi$ on Ω_0, $|\nabla \xi| + \Delta \xi \in L^\infty(\Omega_0)$ and

$$\begin{aligned} &\forall f \in \mathrm{Dom}(T_1), \quad \xi f \in \mathrm{Dom}(t_2), \\ &\forall g \in \mathrm{Dom}(T_2), \quad \xi g \in \mathrm{Dom}(t_1); \end{aligned} \tag{3.11}$$

here we understand ξf as

$$\begin{cases} \xi(x) f(x), & x \in \Omega_2 \cap \Omega_1, \\ 0, & x \in \Omega_2 \setminus \Omega_1, \end{cases} \tag{3.12}$$

and analogously for ξg. ■

An illustration of a choice of suitable cut-off ξ is presented in Figure 3.2. We

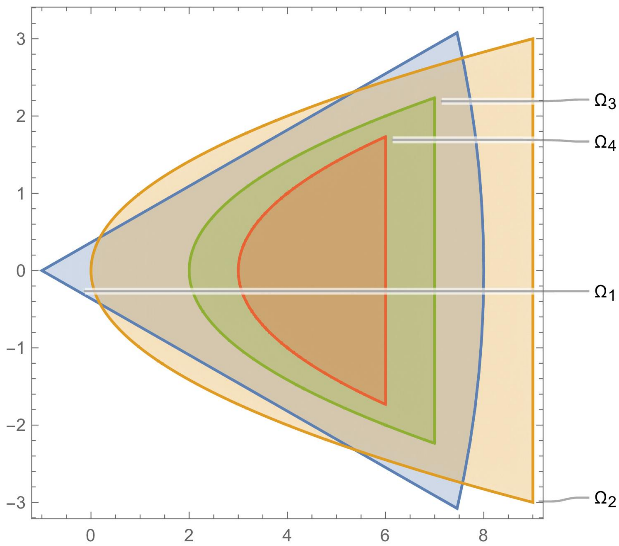

Figure 3.2: The domains Ω_1 (blue) and Ω_2 (yellow) are taken as a part of sector and parabola, respectively. One can construct $\xi \in C^\infty(\Omega_0)$ with $\Omega_0 := \Omega_1 \cup \Omega_2$ such that $\xi = 1$ on $\Omega_4 \subset \Omega_1 \cap \Omega_2$ (orange) and $\xi = 0$ on the complement of Ω_3 (green) in Ω_0. Since $\operatorname{supp} \xi$ is bounded, the conditions (3.11) are satisfied for any admissible Q_1, Q_2 (which is not the case in general for unbounded Ω_1, Ω_2 and unbounded $\operatorname{supp} \xi$).

introduce

$$\widetilde{\xi} := 1 - \xi, \qquad \zeta := \chi_{\operatorname{supp} \widetilde{\xi}} \tag{3.13}$$

where ξ is as in Assumption 3.2.1; see also Figure 3.2. In $L^2(\Omega_0)$, let P_j, P and $\widetilde{P}$ be the following orthogonal projections

$$P_j f = \chi_{\Omega_j} f, \quad P f = \chi_{\Omega_1 \cap \Omega_2} f, \quad \widetilde{P} := I - P, \qquad f \in L^2(\Omega_0). \tag{3.14}$$

From regular perturbation theory [31, Chap. XII.2], [29, Thm. 2] we know that the distance of the eigenvalues of the perturbed operator can be estimated by the norm of the difference of the resolvents. Therefore in this generalized non-self-adjoint setting, we make use of the following theorem

Theorem 3.2.2. *[34, Thm. 3.2] For $j = 1, 2$, let Ω_j, T_j and ξ be as in Assumption 3.2.1, let ζ be as in* (3.13) *and let P_j be as in* (3.14)*. Then there exists a constant $K \geq 0$, depending only on $\|\nabla\xi\|_{L^\infty}$ and $\varepsilon_{\nabla,j}$, $M_{\nabla,j}$, such that*

$$\begin{aligned} &\|R_1(-1)P_1 - R_2(-1)P_2\|_{\mathcal{B}(L^2(\Omega_0))} \\ &\qquad \leq K\left(\left\|\frac{\xi(Q_1-Q_2)}{(Q_1+1)(Q_2+1)}\right\|_{L^\infty(\Omega_1\cap\Omega_2)} + \sum_{j=1}^{2}\left\|\frac{\zeta}{Q_j+1}\right\|_{L^\infty(\Omega_j)}\right). \end{aligned} \tag{3.15}$$

Let T_j, $j = 1, 2$, be as in Assumption 3.2.1 and let $\mu \in \sigma(T_1)$ be an isolated eigenvalue of finite algebraic multiplicity $m \in \mathbb{N}$. If the norm of the difference of resolvents estimated in Theorem 3.2.2), then $\sigma(T_2)$ contains exactly m eigenvalues $\{\mu_k\}_{k=1}^m$ in a neighborhood of μ (counting with multiplicities). This follows by estimating the norm of difference of spectral projections (with a suitable contour γ_μ)

$$E_1 := \frac{1}{2\pi\mathrm{i}}\int_{\gamma_\mu}(z-T_1)^{-1}P_1\,\mathrm{d}z, \qquad E_2 := \frac{1}{2\pi\mathrm{i}}\int_{\gamma_\mu}(z-T_2)^{-1}P_2\,\mathrm{d}z; \tag{3.16}$$

for details see *e.g.* [9, Thm. 5.1], [29], [20, Chap. IV].

Our goal is to estimate the distance of μ and the average of μ_k

$$\hat{\mu} := \frac{1}{m}\sum_{k=1}^{m}\mu_k \tag{3.17}$$

and the distance of eigenfunctions.

Theorem 3.2.3. *[34, Thm. 3.4] For $j = 1, 2$, let Ω_j, T_j and ξ be as in Assumption 3.2.1, let ζ be as in* (3.13)*, let P_j, P and $\widetilde{P}$ be as in* (3.14)*. Let $\mu \in \sigma(T_1)$ be an isolated eigenvalue of finite algebraic multiplicity $m \in \mathbb{N}$. Suppose further that Ω_j and Q_j, $j = 1, 2$, are such that the spectral projections E_j, $j = 1, 2$, in* (3.16) *satisfy $\|E_1 - E_2\| < 1$. Then the following hold.*

i) *Let $\hat{\mu}$ be as in* (3.17)*, then*

$$|\mu - \hat{\mu}| \leq C_{1,\mu}\max_{\substack{\phi\in\mathrm{Ran}(E_1)\\ \|\phi\|=1}}\left\|\frac{\xi(Q_1-Q_2)}{(Q_1+1)(Q_2+1)}\phi\right\| + C_{2,\mu}\max_{\substack{\phi\in\mathrm{Ran}(E_1)\\ \|\phi\|=1}}\|\zeta\phi\|, \tag{3.18}$$

ii) *For all* $\psi \in \operatorname{Ran}(E_1)$*, we have*

$$\|\psi - E_2\psi\| \le D_{1,\mu} \max_{\substack{\phi \in \operatorname{Ran}(E_1) \\ \|\phi\|=1}} \left\| \frac{\xi(Q_1 - Q_2)}{(Q_1+1)(Q_2+1)} \phi \right\| + D_{2,\mu} \max_{\substack{\phi \in \operatorname{Ran}(E_1) \\ \|\phi\|=1}} \|\zeta\phi\| + \|E_2\| \max_{\substack{\phi_2 \in \operatorname{Ran}(E_2) \\ \|\phi_2\|=1}} \|\widetilde{P}\phi_2\|, \tag{3.19}$$

3.3 Sequence of operators

We use Theorems 3.2.2 and 3.2.3 for a sequence of operators $\{T_n\}$ converging to T_∞, in the setting summarized as follows.

Assumption 3.3.1. [34, Asm. 3.5] Suppose that

i) domains $\{\Omega_n\}_{n\in\mathbb{N}^*} \subset \mathbb{R}^d$ are open (non-empty) and $\Omega_n \subset \Omega_\infty$, $n \in \mathbb{N}$;

ii) potentials $Q_n \in W^{1,\infty}_{\mathrm{loc}}(\overline{\Omega_n})$ with $\operatorname{Re} Q_n \ge 0$, $n \in \mathbb{N}^*$, satisfy (3.7) uniformly,

$$\exists \varepsilon_\nabla \in [0, \varepsilon_{\mathrm{crit}}),\ \exists M_\nabla \ge 0,\ \forall n \in \mathbb{N}^*,\ |\nabla Q_n| \le \varepsilon_\nabla |Q_n|^{\frac{3}{2}} + M_\nabla \quad \text{a.e. in } \Omega_n; \tag{3.20}$$

iii) operators $T_n = -\Delta + Q_n$ in $L^2(\Omega_n)$ (introduced via forms t_n, $n \in \mathbb{N}^*$, as in Section 3.1) and cut-offs $\{\xi_n\}_{n\in\mathbb{N}}$ are such that

$$\sup_{n\in\mathbb{N}} \left(\| |\nabla \xi_n| \|_{L^\infty} + \|\Delta \xi_n\|_{L^\infty} \right) < \infty \tag{3.21}$$

and that the conditions of Assumption 3.2.1 are satisfied for Ω_1, Ω_2, ξ, T_1, T_2, t_1, t_2 replaced by Ω_n, Ω_∞, ξ_n, T_n, T_∞, t_n, t_∞, respectively, for every $n \in \mathbb{N}$;

iv) potentials $\{Q_n\}$ converge in the following sense

$$\tau_n := \left\| \frac{\xi_n(Q_n - Q_\infty)}{(Q_n+1)(Q_\infty+1)} \right\|_{L^\infty(\Omega_n)} + \left\| \frac{\zeta_n}{Q_n+1} \right\|_{L^\infty(\Omega_n)} + \left\| \frac{\zeta_n}{Q_\infty+1} \right\|_{L^\infty(\Omega_\infty)} = o(1), \quad n \to \infty, \tag{3.22}$$

where $\widetilde{\xi}_n := 1 - \xi_n$, $\zeta_n := \chi_{\operatorname{supp} \widetilde{\xi}_n}$, $n \in \mathbb{N}$. ■

Note that in the setting of Assumption 3.3.1, the domain Ω_0 in Assumption 3.2.1 corresponds to Ω_∞; the projections P_1, P_2 in (3.14) correspond to

$$P_n := \chi_{\Omega_n} \cdot, \quad P_\infty = I_{L^2(\Omega_\infty)}, \tag{3.23}$$

respectively and the projection P in (3.14) corresponds to P_n. To formulate the result we introduce notation $\{\nu_k\}$ for the isolated eigenvalues of T_∞ with finite algebraic multiplicities $\{m_a(\nu_k)\}$,

$$\sigma_{\mathrm{disc}}(T_\infty) = \{\nu_k\}, \quad m_a(\nu_k) < \infty, \tag{3.24}$$

and for spectral projections of T_∞ and $\{T_n\}$

$$E_k := \frac{1}{2\pi \mathrm{i}} \int_{\gamma_k} (z - T_\infty)^{-1} \, \mathrm{d}z, \qquad E_{k,n} := \frac{1}{2\pi \mathrm{i}} \int_{\gamma_k} (z - T_n)^{-1} P_n \, \mathrm{d}z, \tag{3.25}$$

where $\{\gamma_k\}$ are suitable contours around $\{\nu_k\}$. Moreover, we use notation

$$\kappa_n := \max_{\substack{\phi \in \mathrm{Ran} E_k \\ \|\phi\|=1}} \left(\left\| \frac{\xi_n (Q_n - Q_\infty)}{(Q_n + 1)(Q_\infty + 1)} \phi \right\| + \|\zeta_n \phi\| \right). \tag{3.26}$$

Corollary 3.3.2. *[34, Cor. 3.6] Let Assumption 3.3.1 be satisfied and let P_n, ν_k, E_k, $E_{k,n}$ and κ_n be as in* (3.23), (3.24), (3.25) *and* (3.26). *Then the following hold as $n \to \infty$.*

i) *$\{T_n\}$ converge to T_∞ in the norm resolvent sense (hence there is no spectral pollution): for every $z \in \rho(T_\infty)$, there is $n_z > 0$ such that $z \in \rho(T_n)$, $n > n_z$, and*

$$\|(T_n - z)^{-1} P_n - (T_\infty - z)^{-1}\|_{\mathcal{B}(L^2(\Omega_\infty))} = \mathcal{O}_z(\tau_n); \tag{3.27}$$

ii) *spectral projections converge in norm:*

$$\|E_{k,n} - E_k\|_{\mathcal{B}(L^2(\Omega_\infty))} = \mathcal{O}_k(\tau_n); \tag{3.28}$$

iii) *there is spectral inclusion for isolated eigenvalues with finite algebraic multiplicities: for every $\nu_k \in \sigma_{\mathrm{disc}}(T_\infty)$, as $n \to \infty$, there are exactly $m_a(\nu_k)$ eigenvalues $\mu_{k,n}^{(j)}$, $j = 1, \dots, m_a(\nu_k)$, of T_n in a neighborhood of ν_k (repeated according to their algebraic multiplicities) and*

$$|\nu_k - \hat{\mu}_{k,n}| = \mathcal{O}_k(\kappa_n), \quad \hat{\mu}_{k,n} := \frac{1}{m_a(\nu_k)} \sum_{j=1}^{m_a(\nu_k)} \mu_{k,n}^{(j)}; \tag{3.29}$$

iv) *(generalized) eigenfunctions converge in norm: for very $\psi \in \mathrm{Ran}(E_k)$*

$$\|\psi - E_{k,n}\psi\| = \mathcal{O}_k(\kappa_n), \quad n \to \infty. \tag{3.30}$$

The abstract result of Corollary 3.3.2 will be applied to specific scenarios.

3.4 Strong coupling regime

We consider a family of Dirichlet realizations of

$$T_g = -\Delta + Q_1 + \mathrm{i} g Q_2, \qquad g > 0, \tag{3.31}$$

in $L^2(\Omega)$ where Ω is open, functions Q_i, $i = 1, 2$, are real valued and $g \to +\infty$.

Operators with this structure arise in several contexts, in particular, in enhanced dissipation, see Example 3.4.1, in $\mathcal{PT}$-symmetric phase transitions, see Examples 3.4.2 and 3.4.3, or when $Q_1 = 0$ as semi-classical problems with purely imaginary potentials, see *e.g.* [19, 3, 1], in particular in the context of Bloch-Torrey equation.

We focus here on the case when Ω is (typically) unbounded and $|Q_2|$ has a global minimum inside of Ω, see Assumption 3.4.1 for details. As an application of Corollary 3.3.2, we describe some of the diverging eigenvalues as $g \to +\infty$. We show how Theorem 3.4.3 can be implemented and indicate its possible further extensions.

Assumption 3.4.1. [34, Asm. 7.1.] Let $\Omega \subset \mathbb{R}^d$ be open with $0 \in \Omega$, let $\overline{B_R(0)} \subset \Omega$ for some $R > 0$ and let $Q_1 \in C^1(\overline{\Omega}; \mathbb{R})$ with $Q_1 \geq 0$, $Q_2 \in C^1(\overline{\Omega} \setminus \{0\}; \mathbb{R})$. Suppose further that

i) for some $\varepsilon > 0$, the condition (3.7) is satisfied with Ω replaced by $\Omega \setminus \overline{B_\varepsilon(0)}$ and Q replaced separately by Q_1 and by Q_2;

ii) $Q_2(0) = 0$ and $|Q_2|$ attains the global minimum at 0, *i.e.* for every $\delta > 0$

$$\inf_{x \in \Omega \setminus \overline{B_\delta(0)}} |Q_2(x)| > 0; \tag{3.32}$$

iii) there exists $Q_\infty \in C(\mathbb{R}^d) \cap C^1(\mathbb{R}^d \setminus \{0\}; \mathbb{R})$ with $\min_{|x|=1} |Q_\infty(x)| > 0$ such that for some $\kappa > 0$

$$\begin{aligned} Q_\infty(tx) &= t^\kappa Q_\infty(x), && x \in \mathbb{R}^d,\ t > 0, \\ Q_2(x) - Q_\infty(x) &= |x|^\kappa h_0(x), && h_0(x) = o(1), \quad |x| \to 0, \\ |\nabla Q_2(x) - \nabla Q_\infty(x)| &= |x|^{\kappa-1} h_1(x), && h_1(x) = o(1), \quad |x| \to 0, \end{aligned} \tag{3.33}$$

and the discrete spectrum of $S_\infty := -\Delta + \mathrm{i} Q_\infty$ in $L^2(\mathbb{R}^d)$ is non-empty. ■

Example 3.4.2. Typical examples of S_∞ in Assumption 3.4.1 in one dimension are

$$-\partial_x^2 + \mathrm{i} x^n, \quad n \in \mathbb{N} \setminus \{1\}, \qquad -\partial_x^2 + \mathrm{i}|x|^\kappa, \quad \kappa > 0. \tag{3.34}$$

The spectra of the former for $n = 2k+1$, $k \in \mathbb{N}$, are real, see [35], and the spectra of the remaining operators with even potential can be obtained by complex scaling (after possibly reducing the problem to Dirichlet/Neumann operators in $L^2(\mathbb{R}_+)$). A typical case in more dimensions is an imaginary oscillator with potential $\mathrm{i}\langle Ax, x\rangle_{\mathbb{R}^d}$ and a positive definite matrix A. ■

Theorem 3.4.3. *[34, Thm. 7.3.] Let Assumption 3.4.1 be satisfied and let T_g, $g > 0$, be as in (3.31). Then the spectra of T_g contain asymptotically the eigenvalues (with $k \in \mathbb{N}$ and $j \in \{1, \dots, m_a(\nu_k)\}$)*

$$\lambda_{k,g}^{(j)} = g^{\frac{2}{2+\kappa}} \left(\nu_k + \rho_{k,g}^{(j)}\right), \quad g \to +\infty, \tag{3.35}$$

where $\{\nu_k\} = \sigma_{\mathrm{disc}}(S_\infty)$ and, as $g \to +\infty$, $\rho_{k,g}^{(j)} = o_{j,k}(1)$ and for any $\beta \in (0,1)$,

$$\frac{1}{m_a(\nu_k)} \left| \sum_{j=1}^{m_a(\nu_k)} \rho_{k,g}^{(j)} \right| = \mathcal{O}_k \left(g^{-\frac{\min\{2,\kappa(1-\beta)\}}{2+\kappa}} + \sup_{|y| \le g^{-\frac{\beta}{2+\kappa}}} |h_0(y)| \right). \tag{3.36}$$

3.4.1 Enhanced dissipation

For operators T_g, sufficient conditions for the divergence of the real parts of all eigenvalues of T_g as $g \to +\infty$ were found *cf.* [15, 17, 32]. In [32], the specific operator

$$T_g = -\partial_x^2 + x^2 + \mathrm{i}g(1 + |x|^\kappa)^{-1}, \tag{3.37}$$

in $L^2(\mathbb{R})$ and with $\kappa > 0$ was analyzed and an estimate on the divergence rate of the real part of eigenvalues $\operatorname{Re} \sigma(T_g) \gtrsim g^{\frac{2}{\kappa+2}}$ was proved, *cf.* [32, Thm. 1.2]. Similar problem and result was also established in [17, Thm. 1.9].

Note that the conjugated and shifted operator $T_g^* + \mathrm{i}g$ satisfies Assumption 3.4.1 with $Q_2(x) = |x|^\kappa/(1 + |x|^\kappa)$, $Q_\infty(x) = |x|^\kappa$ and $h_0(x) = -Q_2(x)$. Therefore by Theorem 3.4.3, spectra of T_g contain asymptotically the eigenvalues

$$\lambda_{k,g} = g^{\frac{2}{\kappa+2}} (\overline{\nu_k + \rho_{k,g}}) + \mathrm{i}g, \quad g \to +\infty, \tag{3.38}$$

where $\{\nu_k\}$ are the eigenvalues of operator in (3.34) with the potential $\mathrm{i}|x|^\kappa$. The remainder decays as $\rho_{k,g} = \mathcal{O}(g^{\frac{-\kappa}{2(2+\kappa)}})$ for $\kappa \in (0,4)$ and $\rho_{k,g} = \mathcal{O}(g^{\frac{-2}{2+\kappa}})$ for $\kappa \ge 4$. This result shows that the estimate in [32, Thm. 1.2] is optimal (see Figure 3.1).

3.4.2 $\mathcal{PT}$-symmetric phase transitions I

Let $\Omega = \mathbb{R}$, Q_1 be even, Q_2 odd and such that Assumption 3.4.1 is satisfied. The operators T_g in (3.31) with such Q_1, Q_2 have the antilinear $\mathcal{PT}$-symmetry and so the spectra of T_g consists of complex conjugate pairs. The spectrum of T_0 is real due to the self-adjointness, however, as $g \to \infty$, a graduate appearance of complex conjugated (non-real) spectral points pairs, called $\mathcal{PT}$-symmetric phase transitions, was observed in many examples, see *e.g.* [38] for one of the first works.

For $Q_1(x) = x^2$, upper estimates on the number of non-real eigenvalues are given in [24] and precise spectral analysis of the double δ potential (with a fixed $b > 0$)

$$-\partial_x^2 + x^2 + \mathrm{i}g(\delta(x-b) - \delta(x+b)) \tag{3.39}$$

is performed in [26, 6]. In particular it is showed in [6] that the number of non-real eigenvalues of (3.39) diverges as $g \to +\infty$.

We consider here

$$T_g = -\partial_x^2 + x^2 + \mathrm{i}gx^3\mathrm{e}^{-x^2}, \tag{3.40}$$

in $L^2(\mathbb{R})$ which can be viewed as a "smooth version" of (3.39). In this case, we can apply Theorem 3.4.3 in three stationary points of $Q_2(x) = x^3\mathrm{e}^{-x^2}$, namely, $x_0 = 0$, $x_1 = -\sqrt{3/2}$ and $x_2 = -x_1$.

The operator T_g satisfies Assumption 3.4.1 with $Q_1(x) = x^2$, $Q_2(x) = x^3\mathrm{e}^{-x^2}$, $Q_\infty(x) = x^3$, $\kappa = 3$, $h_0(x) = \mathrm{e}^{-x^2} - 1$. Therefore the eigenvalues

$$\lambda_{k,g}^{(x_0)} = g^{\frac{2}{5}}(\nu_k + \mathcal{O}_k(g^{-\frac{6}{25}})), \quad g \to +\infty, \tag{3.41}$$

where ν_k are (real) eigenvalues of the imaginary cubic oscillator (the potential $\mathrm{i}x^3$), *cf.* Example 3.4.2, lie asymptotically in the spectra of T_g.

Further sets of eigenvalues can be obtained by applying the Theorem 3.4.3 to the operator $\widetilde{T}_g - \mathrm{i}g(3/(2\mathrm{e}))^{\frac{3}{2}}$, where $\widetilde{T}_g$ is the operator obtained from T_g by the translation $x \mapsto x + x_1$. It satisfies the Assumption 3.4.1 with $\kappa = 2$ and

$$\begin{aligned} Q_1(x) &= (x+x_1)^2, \quad Q_2(x) = (x+x_1)^3\mathrm{e}^{-(x+x_1)^2} + (\tfrac{3}{2\mathrm{e}})^{\frac{3}{2}}, \\ Q_\infty(x) &= (\tfrac{27}{2\mathrm{e}^3})^{\frac{1}{2}}x^2, \quad h_0(x) = \frac{Q_2(x)}{x^2} - (\tfrac{27}{2\mathrm{e}^3})^{\frac{1}{2}}. \end{aligned} \tag{3.42}$$

Therefore the eigenvalues

$$\lambda_{k,g}^{(x_1)} = g^{\frac{1}{2}}(\nu_k + \mathcal{O}_k(g^{-\frac{1}{8}})) - \mathrm{i}g(2\mathrm{e})^{-\frac{1}{2}} + \tfrac{3}{2}, \quad g \to +\infty, \tag{3.43}$$

where $\nu_k = (\frac{27}{2\mathrm{e}^3})^{\frac{1}{4}}\mathrm{e}^{\mathrm{i}\frac{\pi}{4}}(2k+1)$, $k \in \mathbb{N}_0$, lie asymptotically in the spectra of T_g. Analogous steps can be implemented on the conjugate operator T_g^* and we obtain the second set of eigenvalues $\lambda_{k,g}^{(x_2)} = \overline{\lambda_{k,g}^{(x_1)}}$, *cf.* Figure 3.3.

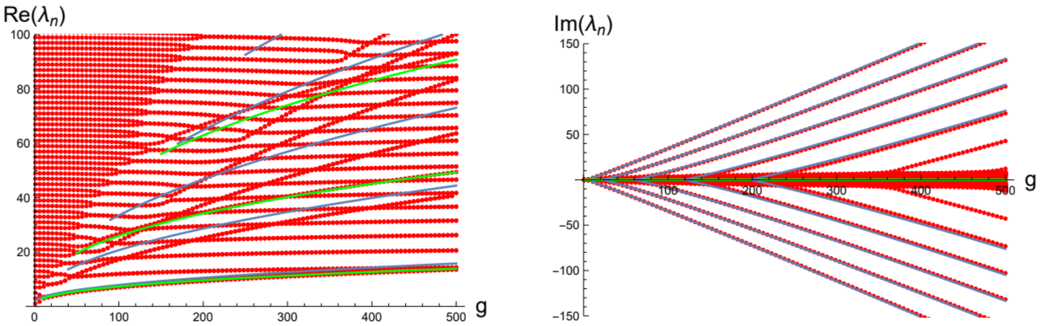

Figure 3.3: $Q_1(x) = x^2$, $Q_2(x) = x^3 e^{-x^2}$: Real (left) and imaginary (right) part of the eigenvalues (red) of operators T_g with $g = 5, 10, \ldots, 500$. Asymptotic curves (blue) $\lambda_{k,g}^{(x_1)}, \lambda_{k,g}^{(x_2)}$ and (green) $\lambda_{k,g}^{(x_0)}$ for $k = 1, 2, \ldots, 5$.

3.4.3 $\mathcal{PT}$-symmetric phase transitions II

$\mathcal{PT}$-symmetric phase transitions were studied in [12] for operators in $L^2(\mathbb{R})$ with polynomial potentials

$$- \partial_x^2 + \frac{x^{2M}}{2M} + \mathrm{i}g\frac{x^{M-1}}{M-1}, \quad M \in 2\mathbb{N}, \tag{3.44}$$

and the eventual transition of each eigenvalue was established, see [12, Thm. 1.1] for precise claims.

For $M \geq 4$, Theorem 3.4.3 used for the stationary point of Q_2 at $x_0 = 0$ yields that spectra of operators (3.44) contain asymptotically the eigenvalues

$$\lambda_{k,g,M}^{(x_0)} = g^{-\frac{2}{M+1}}(\nu_{k,M} + \mathcal{O}(g^{-\frac{2}{M+1}})), \quad g \to +\infty, \tag{3.45}$$

where $\nu_{k,M} = (\frac{1}{M-1})^{\frac{2}{M+1}}\mu_{k,M}$, and $\{\mu_{k,M}\}_k$ are (positive) eigenvalues of $-\partial_x^2 + \mathrm{i}x^{M-1}$, see Example 3.4.2. Notice that the leading term of the asymptotic expansion of these eigenvalues is real and also that no such sequence is obtained for $M = 2$ when $Q_2(x) = x$ since the spectrum of imaginary Airy operator is empty. Nonetheless, the (diverging) non-real eigenvalues found in [12] are clearly visible in Figure 3.4 for $M = 2$ and in similar plots for higher M. To obtain asymptotics of these we use other stationary points of the potential outside real axis.

Consider first a simpler shifted oscillator $-\partial_x^2 + x^2 + 2\mathrm{i}gx$ where Theorem 3.4.3 is not applicable for the stationary point $x_0 = 0$ directly either. Nevertheless, writing $x^2 + 2\mathrm{i}gx = (x + \mathrm{i}g)^2 + g^2$ and the complex shift $x \mapsto x - \mathrm{i}g$, *i.e.* to the complex stationary point $x_1 = -\mathrm{i}g$, reveals the well-known diverging eigenvalues $\{2k+1+g^2\}_{k\in\mathbb{N}_0}$. Notice that the complex shift leaves the spectrum invariant by an argument similar to complex scaling.

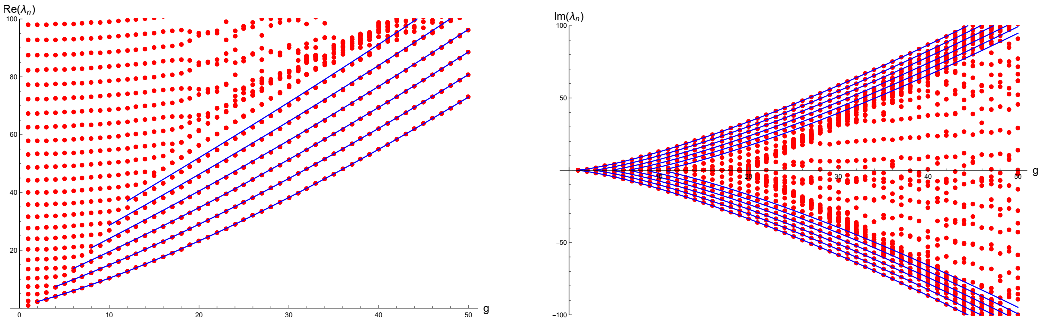

Figure 3.4: $Q_1(x) = x^4/4$, $Q_2(x) = x$: Real (left) and imaginary (right) part of the eigenvalues (red) of operators T_g in (3.48) with $g = 5, 10, \ldots, 500$. Asymptotic curves (blue) for $\lambda_{k,g}^{(x_2)}$, $\lambda_{k,g}^{(x_3)}$ with $k = 1, 2, \ldots, 5$.

Namely, the shift $x \mapsto x + \theta$ generates a holomorphic family (in θ) of operators of type A since the operator domains are constant, moreover, for $\theta \in \mathbb{R}$, the spectra stay clearly invariant (such shifts induce a unitary transform).

For operators (3.44), we first rescale $x \mapsto g^{2M/(M+1)}x$ to obtain

$$\frac{1}{g^{\frac{2}{M+1}}}\left[-\partial_x^2 + g^2\left(\frac{x^{2M}}{2M} + \mathrm{i}\frac{x^{M-1}}{M-1}\right)\right] \tag{3.46}$$

The stationary points of the potential read

$$x_0 = 0, \qquad x_k = \mathrm{e}^{\mathrm{i}\frac{4k-1}{2(M+1)}\pi}, \quad k = 1, \ldots, M+1. \tag{3.47}$$

In particular for $M = 2$, besides $x_0 = 0$, which was already covered above, we have $x_1 = \mathrm{i}$, $x_2 = \mathrm{e}^{\mathrm{i}\frac{7}{6}\pi}$ and $x_3 = \mathrm{e}^{\mathrm{i}\frac{11}{6}\pi}$. The shift to x_3 leads to the operator

$$T_g = \frac{1}{g^{\frac{2}{3}}}\left(-\partial_x^2 + \frac{g^2}{4}\left[x^2(x+\sqrt{3})^2 - \mathrm{i}x^2(2x + 3\sqrt{3})\right] + \frac{3}{4}g^2\mathrm{e}^{\mathrm{i}\frac{\pi}{3}}\right) \tag{3.48}$$

which is not directly covered by Theorem 3.4.3 as g^2 multiplies the whole potential. Nonetheless, Theorem 3.4.3 can be generalized in a straightforward way if the real part of the potential is non-negative and it yields that eigenvalues

$$\lambda_{k,g}^{(x_3)} = \sqrt{\frac{3}{2}}g^{\frac{1}{3}}(\nu_k + \mathcal{O}_k(g^{-\frac{1}{6}})) + \frac{3}{4}\mathrm{e}^{\mathrm{i}\frac{5\pi}{3}}g^{\frac{4}{3}}, \quad \lambda_{k,g}^{(x_2)} = \overline{\lambda_{k,g}^{(x_3)}}, \quad g \to +\infty, \tag{3.49}$$

where $\nu_k = \mathrm{e}^{\mathrm{i}\frac{\pi}{6}}(2k+1)$, $k \in \mathbb{N}_0$, lie asymptotically in the spectra of T_g, see Figure 3.4 for illustration. The shift to x_1 gives the potential with the quadratic term $-3x^2/2$ which does not correspond to a suitable limit operator.

The situation is more complicated for $M > 2$, there are more stationary points and in general the real part of the potential after the shift is not non-negative (although bounded from below). Moreover, numerics suggests that only two stationary points lead to diverging eigenvalues. Namely the points for $k = \frac{M}{2} + 1$ and $k = M + 1$, *i.e.* $\mathrm{e}^{\mathrm{i}\frac{2M+3}{2M+2}}$ and $\mathrm{e}^{\mathrm{i}\frac{4M+3}{2M+2}}$ (the points where the shifted potential has a global extreme of imaginary part).

Chapter 4

Domain truncations of Schrödinger operators

It was established in [9] that for potentials Q with $\operatorname{Re} Q \geq 0$, $|Q(x)| \to +\infty$ as $|x| \to \infty$ and satisfying suitable regularity conditions, the domain truncation approximation technique is spectrally exact, *i.e.* all eigenvalues of $T_\infty = -\Delta + Q(x)$ acting on $L^2(\Omega)$ are approximated by eigenvalues of truncated operators $T_n = -\Delta + Q(x)$ acting on $L^2(\Omega_n)$ where $\{\Omega_n\}$ exhausts Ω in the limit $n \to \infty$, and there is no pollution (there are no finite accumulation points of eigenvalues of $\{T_n\}$ which are not eigenvalues of T_∞), see *e.g.* [11].

We apply Corollary 3.3.2 to domain truncations of a given Schrödinger operator with the underlying initial domain $\mathbb{R}^d$ to bounded expanding domains $\{\Omega_n\}$. It is easy to verify that the results can be reformulated for other initial domains like exterior domains in $\mathbb{R}^d$, cones in $\mathbb{R}^d$ etc.

Assumption 4.0.1. Let $\Omega_\infty := \mathbb{R}^d$, let $\{\Omega_n\} \subset \mathbb{R}^d$ be bounded and open sets and let there exist a sequence $\{r_n\} \subset (0, \infty)$ such that $r_n \nearrow +\infty$ and

$$B_{r_n+2}(0) \subset \Omega_n, \qquad n \in \mathbb{N}. \tag{4.1}$$

Let Q_∞ satisfy Assumption 3.1.1 (with $Q := Q_\infty$) and suppose in addition that

$$\lim_{R\to\infty} \operatorname*{ess\,inf}_{|x|>R, x\in\Omega} |Q_\infty(x)| = +\infty. \tag{4.2}$$

■

Theorem 4.0.2. *Let Assumption 4.0.1 be satisfied and let T_n be the Dirichlet realizations of $-\Delta + Q$ in $L^2(\Omega_n)$, $n \in \mathbb{N}^*$, respectively. Then the statements of Corollary 3.3.2 hold with $\{\nu_k\} := \sigma(T_\infty)$ and*

$$\tau_n = \left\| \widetilde{\chi}_{B_{r_n}(0)} |Q|^{-1} \right\|_{L^\infty}, \quad \kappa_n = \max_{\substack{\phi \in \operatorname{Ran} E_k \\ \|\phi\|=1}} \|\widetilde{\chi}_{B_{r_n}(0)} \phi\|_{L^2}, \quad n \in \mathbb{N}. \tag{4.3}$$

Our results are applicable for truncations of operators T without compact resolvent to suitable unbounded domains. Roughly speaking, one can truncate the parts of domain where the potential Q is unbounded as $x \to \infty$.

4.1 Diverging eigenvalues in domain truncations

Even though domain truncation is spectrally exact, it does not exclude possible existence of further eigenvalues in the spectra of truncated operators, provided they escape to infinity as $n \to \infty$. This phenomenom of diverging eigenvalues is common on certain types of open domains with corners (such as bounded interval) and dominant imaginary part of the potential Q.

To identify the diverging eigenvalues, a combination of suitable unitary transforms (translation and scaling) is performed, following the ideas in [7, Thm. 3.1]. This procedure explained in the model case in Example 4.1.1 reveals a suitable limiting operator and hence asymptotic formulas for diverging eigenvalues.

Example 4.1.1 (Imaginary Airy operator)**.** Consider $\Omega_n := (-s_n, s_n)$ with some $\{s_n\} \subset \mathbb{R}_+$ with $s_n \nearrow +\infty$ and

$$T_n = -\partial_x^2 + \mathrm{i}x, \quad \mathrm{Dom}(S_n) = W^{2,2}(\Omega_n) \cap W_0^{1,2}(\Omega_n). \tag{4.4}$$

The translation $x \mapsto x - s_n$ leads to unitarily equivalent operators

$$-\partial_x^2 + \mathrm{i}x - \mathrm{i}s_n =: S_n - \mathrm{i}s_n, \quad \mathrm{Dom}(S_n) = W^{2,2}(\Sigma_n) \cap W_0^{1,2}(\Sigma_n), \tag{4.5}$$

where $\Sigma_n = (0, 2s_n)$. Theorem 4.0.2 implies that S_n converges to $S_{\mathrm{A}} = -\partial_x^2 + \mathrm{i}x$ in $L^2(\mathbb{R}_+)$ in the norm resolvent convergence sense, hence the approximation is spectrally exact and so the spectra of S_n contain asymptotically the eigenvalues $\{\nu_k + \rho_{k,n}\}_k$ where $\sigma(S_{\mathrm{A}}) = \{\nu_k\} = \{\mathrm{e}^{-\mathrm{i}\frac{2\pi}{3}} a_k\}$, where a_k satisfy $\mathrm{Ai}(a_k) = 0$ as in Section 1.2.1, and with some $c_k > 0$ we have $\rho_{k,n} = \mathcal{O}_k(\exp(-c_k s_n^{3/2}))$ as $n \to \infty$. Thus, by spectral mapping and (4.5), we obtain that spectra of T_n contain asymptotically the eigenvalues

$$\lambda_{k,n} = (\nu_k + \rho_{k,n}) - \mathrm{i}s_n, \quad k \in \mathbb{N}. \tag{4.6}$$

A second set of diverging eigenvalues of T_n can be obtained by two transformations $x \mapsto x + s_n$ and $x \mapsto -x$. Isospectral partner of (4.4) in $L^2(\Sigma_n)$ then takes the form $-\partial_x^2 - \mathrm{i}x + \mathrm{i}s_n$, which is the adjoint operator of (4.5). Hence its spectrum contains asymptotically the conjugate eigenvalues $\{\overline{\lambda_{k,n}}\}$.

In summary, the spectrum of T_n contains asymptotically the complex conjugated eigenvalues $\{\lambda_{k,n}, \overline{\lambda_{k,n}}\}$, *cf.* Figure 4.1. ■

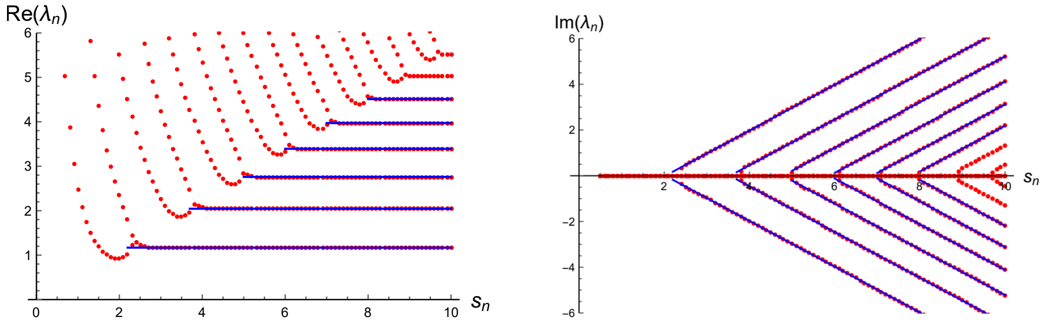

Figure 4.1: Real (left) and imaginary (right) parts of eigenvalues of domain truncations of imaginary Airy operator $-\partial_x^2 + \mathrm{i}x$ in $L^2(\mathbb{R})$ to $L^2((-s_n, s_n))$, $s_n = 0.1n$, $n = 5, 6, \dots, 100$; subject to Dirichlet boundary conditions. Six asymptotic curves (blue) to which the eigenvalues converge; see Example 4.1.1.

In one dimensional case and when Q is imaginary, we give explicit conditions on Q which guarantee the occurence of diverging eigenvalues. To avoid working with conditions at $-\infty$ we express Q in a specific way in terms of a new function U, namely as

$$Q(x) = -\mathrm{i}U(-x), \quad x \in \mathbb{R}. \tag{4.7}$$

Assumption 4.1.2. Let $U \in C^1(\mathbb{R};\mathbb{R}) \cap C^2((x_0, \infty))$ with a sufficiently large $x_0 > 0$ as below satisfy the condition (3.7) on $\mathbb{R}$ with an abitrarily small $\varepsilon_\nabla > 0$ (where we replace Q by U). Let $\Omega_n = (-s_n, t_n)$ with $s_n \nearrow +\infty$ and

$$\lim_{n\to\infty} (s_n + t_n)\sigma_n^{-1} = +\infty, \tag{4.8}$$

where $\sigma_n := |U(s_n)|^{-\frac{1}{3}}$. Suppose further that

i) U is eventually increasing and unbounded at $+\infty$:

$$U'(x) > 0, \quad x > x_0, \qquad \lim_{x\to+\infty} U(x) = +\infty; \tag{4.9}$$

ii) U has controlled derivatives: there is $\nu \geq -1$ such that

$$U'(x) \lesssim U(x)x^\nu, \qquad |U''(x)| \lesssim U'(x)x^\nu, \qquad x > x_0, \tag{4.10}$$

iii) U grows sufficiently fast at $+\infty$:

$$\Upsilon(x) := \frac{x^\nu}{U'(x)^{\frac{1}{3}}} \to 0, \quad x \to +\infty \tag{4.11}$$

iv) U is relatively smaller on $(-\infty, x_0)$: there exists $\delta_0 \in (0,1)$ such that

$$\sup_{y \in (s_n - x_0, s_n + t_n)} U(s_n - y) \leq (1 - \delta_0) U(s_n), \quad n \to \infty. \tag{4.12}$$

■

By Gronwalls inequality, (4.10) implies that for all sufficiently large $x > 0$

$$U(x) \lesssim \begin{cases} x^\gamma, & \nu = -1, \\ \exp(\gamma x^{\nu+1}), & \nu > -1. \end{cases} \tag{4.13}$$

with some $\gamma > 0$. Moreover, there exist constants $c_1, c_2 > 0$ such that for all sufficiently large $x > 0$ and for all $|\delta| \leq \frac{1}{4}|x|^{-\nu}$, we have

$$c_1 U^{(j)}(x) \leq U^{(j)}(x + \delta) \leq c_2 U^{(j)}(x), \qquad j = 0, 1; \tag{4.14}$$

for details see [23, Sec. 3.1] and [25, Sec. 2].

Theorem 4.1.3. *[34, Thm. 5.7] Let Assumption 4.1.2 be satisfied, let Q, U be as in* (4.7) *and let*

$$\sigma_n = U'(s_n)^{-\frac{1}{3}}. \tag{4.15}$$

Then the spectra of Dirichlet realizations $T_n = -\partial_x^2 + Q$ in $L^2(\Omega_n)$, $n \in \mathbb{N}$, contain asymptotically as $n \to \infty$ the eigenvalues

$$\lambda_{k,n} = U'(s_n)^{\frac{2}{3}} \left(\nu_k + \rho_{k,n}\right) - \mathrm{i}U(s_n), \quad \rho_{k,n} = \mathcal{O}_k\big(\Upsilon(s_n) + \exp(-c_k r_n^{\frac{3}{2}})\big), \tag{4.16}$$

where $r_n = (s_n + t_n)\sigma_n^{-1} - 2$.

In the next step, we determine a class of admissible perturbations of U as in Assumption 4.1.2.

Proposition 4.1.4. *[34, Prop. 5.8] Let Assumption 4.1.2 be satisfied. Suppose that $U_1 \in L^\infty_{\mathrm{loc}}(\mathbb{R}; \mathbb{C})$, $U_1' \in L^\infty_{\mathrm{loc}}((x_1, \infty); \mathbb{C})$ for some $x_1 > 0$ and (using notation of Assumption 4.1.2),*

$$U_1'(x) = o(U'(x)), \quad x \to +\infty, \quad \|U_1\|_{L^\infty((-t_n, s_n))} = o(U(s_n)), \tag{4.17}$$

Then, with σ_n as in (4.15)*, the claim of Theorem 4.1.3 remains valid with*

$$\begin{aligned} \lambda_{k,n} &= U'(s_n)^{\frac{2}{3}} \left(\nu_k + \rho'_{k,n}\right) - \mathrm{i}U(s_n) - U_1(s_n), \\ \rho'_{k,n} &= \mathcal{O}_k\big(\Upsilon(s_n) + \iota'_n + \exp(-c_k r_n^{\frac{3}{2}})\big). \end{aligned} \tag{4.18}$$

In particular if the support of U_1 is bounded, then

$$\iota'_n = \mathcal{O}(U(s_n)^{-1} \Upsilon(s_n) s_n^{\nu - 1}), \quad n \to \infty. \tag{4.19}$$

4.2 Odd imaginary potentials

Let $U : \mathbb{R} \to \mathbb{R}$ be odd and satisfy Assumption 4.1.2; note that (4.12) holds automatically if the previous conditions are satisfied. We consider Dirichlet realizations $T_n = -\partial_x^2 + \mathrm{i}U$ in $L^2((-s_n, s_n))$ with $s_n \nearrow +\infty$. Since U is odd, (4.7) corresponds to the relation $Q = \mathrm{i}U$, thus by Theorem 4.1.3, the spectra of T_n contain asymptotically the eigenvalues $\{\lambda_{k,n}\}_k$ in (4.16). Due to the antilinear symmetry of T_n ($x \mapsto -x$ together with complex conjugation, the so-called $\mathcal{PT}$-symmetry), the spectra of T_n contain also $\{\overline{\lambda_{k,n}}\}_k$.

In particular, $U(x) = \operatorname{sgn}(x)|x|^\alpha$ with $\alpha > 0$, satisfies Assumption 4.1.2 with $\nu = -1$ and a possible lack of differentiability of U at 0 can be treated by splitting $U = \eta U + (1-\eta)U$ with $\eta \in C_0^\infty((-2,2))$ and $\eta = 1$ on $(-1,1)$. Notice that $U_1 = \eta U$ satisfies assumptions of Proposition 4.1.4. Hence we obtain

$$\lambda_{k,n} = \alpha^{\frac{2}{3}} s_n^{\frac{2(\alpha-1)}{3}} \left(\nu_k + \mathcal{O}_k\left(s_n^{-\frac{2+\alpha}{3}} \right) \right) - \mathrm{i} s_n^\alpha, \tag{4.20}$$

and their complex conjugates; see Figures 4.1 and 4.2 for illustration in two well-known special cases (the imaginary Airy operator and imaginary cubic oscillator).

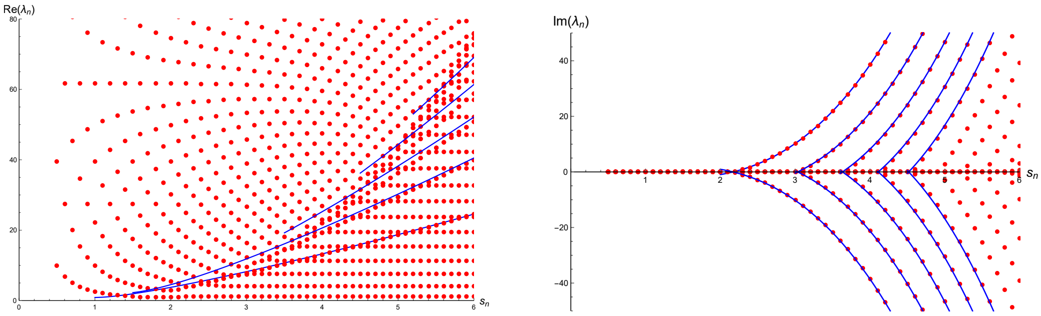

Figure 4.2: $Q(x) = \mathrm{i}x^3$: Real (left) and imaginary (right) part of the eigenvalues (red) of truncated operators T_n, defined on $L^2((-s_n, s_n))$ with $s_n = 0.1n$, $n = 5, 6, \ldots, 60$. Asymptotic curves (blue) for $\lambda_{k,n}$, $\overline{\lambda_{k,n}}$ with first corrections for $k = 1, 2, \ldots, 5$.

In Figure 4.2 we plot the asymptotic curves taking into account the first correction with $\psi_k(y) = \mathrm{Ai}(e^{\frac{\mathrm{i}\pi}{6}} y + \mu_k)$

$$R_{1,n,k} = \frac{\langle (\mathrm{i}\sigma_n^2 (U(s_n) - U(s_n - \sigma_n y) - \mathrm{i}y)\psi_k, \psi_k^* \rangle_{L^2(\mathbb{R}_+)}}{\langle \psi_k, \psi_k^* \rangle_{L^2(\mathbb{R}_+)}}, \tag{4.21}$$

Specifically for $\alpha = 3$

$$R^{(1)}_{1,n,k} = \frac{(\mathrm{i}(-3^{-\frac{1}{3}} s_n^{-\frac{5}{3}} y^2 + 3^{\frac{1}{3}} s_n^{-\frac{10}{3}} y^3)\psi_k, \psi_k^*)_{L^2(\mathbb{R}_+)}}{(\psi_k, \psi_k^*)_{L^2(\mathbb{R}_+)}}, \quad R^{(2)}_{1,n,k} = \overline{R^{(1)}_{1,n,k}} \tag{4.22}$$

The corrected asymptotic formula then holds

$$\lambda^{(1)}_{k,n} = 3^{\frac{2}{3}} s_n^{\frac{4}{3}} \nu_k - \mathrm{i} s_n^3 + \mathrm{i} 3^{\frac{1}{3}} s_n^{-\frac{1}{3}} R_k^a - \mathrm{i} s_n^{-2} R_k^b + s_n^{\frac{4}{3}} \widetilde{r}_{k,n}, \quad \lambda^{(2)}_{k,n} = \overline{\lambda^{(1)}_{k,n}}, \tag{4.23}$$

where

$$R_k^a = \frac{\int_0^\infty y^2 \psi_k^2 \mathrm{d}y}{\int_0^\infty \psi_k^2 \mathrm{d}y}, \quad R_k^b = \frac{\int_0^\infty y^3 {\psi_k}^2 \mathrm{d}y}{\int_0^\infty \psi_k^2 \mathrm{d}y}. \tag{4.24}$$

The case $\alpha = 2j+1$, $j \in \mathbb{N}$ was thoroughly studied in [18], diverging eigenvalues were described by means of spectral scaling graphs, using the methods of analytic WKB and Stokes graph analysis.

4.3 Even imaginary potentials

Let $V : \mathbb{R} \to \mathbb{R}$ be an even and with $V'(x) > 0$ for $x > 0$ and consider Dirichlet realizations $T_n = -\partial_x^2 + \mathrm{i}V$ in $L^2((-s_n, s_n))$ with $s_n \nearrow +\infty$. Theorem 4.1.3 is not directly applicable because of the condition (4.12). Nonetheless, due to the symmetry of V, eigenfunctions of T_n satisfy either Dirichlet or Neumann boundary conditions at 0. Therefore we can split the spectral problem and analyze separately the spectra of

$$\begin{aligned} T_n^{\mathrm{DD}} &= -\partial_x^2 + \mathrm{i}V(x), \quad \mathrm{Dom}(T_n^{\mathrm{DD}}) = W^{2,2}((-s_n,0)) \cap W_0^{1,2}((-s_n,0)), \\ T_n^{\mathrm{DN}} &= -\partial_x^2 + \mathrm{i}V(x), \quad \mathrm{Dom}(T_n^{\mathrm{DN}}) = \{f \in W^{2,2}((-s_n,0)) \,:\, f'(0) = f(-s_n) = 0\}. \end{aligned}$$

Introducing $U := V\chi_{\mathbb{R}_+}$, we obtain that $(T_n^{\mathrm{DD}})^* = -\partial_x^2 + Q$ in $L^2((-s_n, 0))$ with $Q(x) = -\mathrm{i}U(-x)$ as in (4.7).

We assume that this U satisfies Assumption 4.1.2, possibly with perturbations as in Example 4.2, and notice that (4.12) is satisfied automatically. Then Theorem 4.1.3 yields that the spectra of T_n^{DD} contain asymptotically the eigenvalues

$$\lambda^{\mathrm{DD}}_{k,n} = V'(s_n)^{\frac{2}{3}} \left(\overline{\nu_k} + \rho^{\mathrm{DD}}_{k,n} \right) + \mathrm{i}V(s_n), \quad n \to \infty. \tag{4.25}$$

It is not difficult to see that the claim of Theorem 4.1.3 holds also for Neumann boundary conditions at the endpoints as well as for the combinations of Dirichlet and Neumann boundary conditions. Depending on the boundary condition at 0, the limiting operator is Dirichlet or Neuman imaginary Airy operator in $L^2(\mathbb{R}_+)$, in the Neumann case with eigenvalues $\{\nu_k'\} = \{e^{i(\frac{2\omega}{3}-\pi)}\mu_k'\}$ where $\{\mu_k'\}$ are zeros of Ai'. Thus we obtain that the spectra of T_n^{ND} contain asymptotically the eigenvalues

$$\lambda_{k,n}^{\mathrm{DN}} = V'(s_n)^{\frac{2}{3}}\left(\overline{\nu_k} + \rho_{k,n}^{\mathrm{ND}}\right) + iV(s_n), \quad n \to \infty. \tag{4.26}$$

These two sets of eigenvalues have the same main asymptotic terms, however, the corresponding eigenfunctions of T_n are very different (odd and even).

4.4 Imaginary exponential potential with non-empty essential spectrum

Consider the operator $T = -\partial_x^2 + ie^x$ and its truncations T_n to $(-\infty, s_n)$ with $s_n \nearrow +\infty$. Defining $U(x) := e^x$ and $Q(x) := -iU(-x)$ as in (4.7), we obtain that T_n^* is unitarily equivalent via the reflection $x \mapsto -x$ to $-\partial_x^2 + Q$ in $L^2((-s_n, \infty))$. This U satisfies Assumption 4.1.2 with $t_n = +\infty$ and $\nu = 0$, thus by Theorem 4.1.3, the spectra of T_n contain asymptotically the eigenvalues

$$\lambda_{k,n} = e^{\frac{2}{3}s_n}\left(\overline{\nu_k} + \mathcal{O}_k\left(e^{-\frac{1}{3}s_n}\right)\right) + ie^{s_n}, \quad n \to \infty. \tag{4.27}$$

In fact, since Assumption 4.1.2 is satisfied also with $t_n = s_n$, the eigenvalues (4.27), with possibly different remainders, are asymptotically contained in the spectra of operators $T_n = -\partial_x^2 + ie^x$ subject to Dirichlet boundary conditions in $L^2((-s_n, s_n))$; spectra of these are illustrated in Figure 4.3.

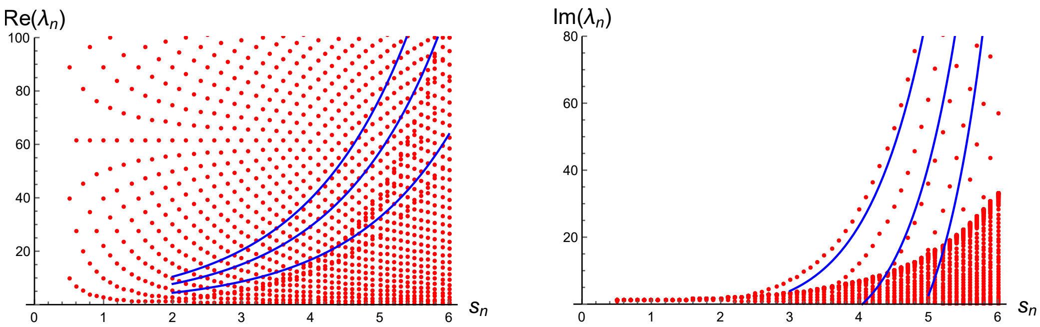

Figure 4.3: $U(x) = ie^x$: Real (left) and imaginary (right) part of the eigenvalues (red) of truncated operators T_n, defined on $L^2((-s_n, s_n))$ with $s_n = 0.1n$, $n = 5, 6, \ldots, 60$. Asymptotic curves (blue) for $\lambda_{k,n}$ with first correction for $k = 1, 2, 3$.

4.5 Radially symmetric potentials on annuli

Consider the exterior domain $\Omega = \mathbb{R}^d \setminus \overline{B_1(0)}$, a radial potential $V : \Omega \to \mathbb{C}$ satisfying Assumption 3.1.1 (with Q replaced by V) and the Dirichlet realization of $T = -\Delta + V$ in $L^2(\Omega)$. Consider also the truncated operators $T_n = -\Delta + V$ in $L^2(\Omega_n)$ with $\Omega_n = \Omega \cap B_{s_n}(0)$ and $s_n \nearrow +\infty$, subject to Dirichlet boundary conditions both on $\partial B_1(0)$ and $\partial B_{s_n}(0)$. Truncations of a specific problem of this type were originally considered in [11] and it was shown in [9, Sec. 6] that such domain truncation is spectrally exact, see also Theorem 4.0.2. Our aim here is to investigate the diverging eigenvalues.

We transform T_n in spherical coordinates with $r \in (1, s_n)$, $\Theta \in \mathcal{S}^{d-1}$, employ the usual unitary transform in the radial part (see *e.g.* [37, Chap. 18])

$$L^2(\mathbb{R}_+; r^{d-1}\mathrm{d}r) \to L^2(\mathbb{R}_+, \mathrm{d}r) \, : \, h(r) \mapsto r^{(d-1)/2} h(r), \tag{4.28}$$

and use the spherical harmonics $\{Y_{l,j}\}_{j=1}^{N(l,d)}$, $l \in \mathbb{N}_0$, $N(l,d) = \frac{(2l+d-2)(l+d-3)!}{l!(d-2)!}$ in $d-1$ dimensions, which satisfy $-\Delta_{\mathcal{S}^{d-1}} Y_{l,j}(\Theta) = l(l+d-2) Y_{l,j}(\Theta)$. Thereby we obtain a decomposition of T_n to one dimensional operators

$$T_{n,l} := -\partial_r^2 + \mathrm{i}U(r) + U_1(r), \quad \mathrm{Dom}(T_{n,l}) := W^{2,2}((1, s_n)) \cap W_0^{1,2}((1, s_n)), \tag{4.29}$$

where $U(r) = V(x)$ for $|x| = r$ and

$$U_1(r) = \frac{(d-1)(d-3) + 4l(l+d-2)}{4r^2}. \tag{4.30}$$

Similarly as in Examples 4.3, 4.4, $T_{n,l}^*$ is unitarily equivalent via the reflection $r \mapsto -r$ to $-\partial_r^2 + Q$ in $L^2((-s_n, -1))$ with $Q(r) = -\mathrm{i}U(-r) - U_1(-r)$.

We suppose that $U\chi_{[1,+\infty]}$ satisfies Assumption 4.1.2 (with perturbations as in Example 4.2) and note that U_1 satisfies conditions of Proposition 4.1.4. Then Theorem 4.1.3 and Proposition 4.1.4 yield that the spectra of $T_{n,l}$ in (4.29) contain asymptotically the eigenvalues

$$\lambda_{k,n,l} = U'(s_n)^{\frac{2}{3}} \left(\overline{\nu_k} + \rho_{k,n,l}\right) + \mathrm{i}U(s_n) - U_1(s_n), \quad n \to \infty. \tag{4.31}$$

In particular for $V(x) = \mathrm{i}|x|^2$ with $x \in \mathbb{R}^d \setminus \overline{B_1(0)}$; a similar potential was originally considered in [11, Sec. 3.1]. From (4.31) we obtain that the spectral of the one dimensional operators $T_{n,l}$, see (4.29), contain asymptotically the eigenvalues

$$\lambda_{k,n,l} = (2s_n)^{\frac{2}{3}} \left(\overline{\nu_k} + \mathcal{O}_{k,l}\left(s_n^{-\frac{4}{3}}\right)\right) + \mathrm{i}s_n^2, \quad n \to \infty; \tag{4.32}$$

Figures 4.4 and 1 illustrate this result.

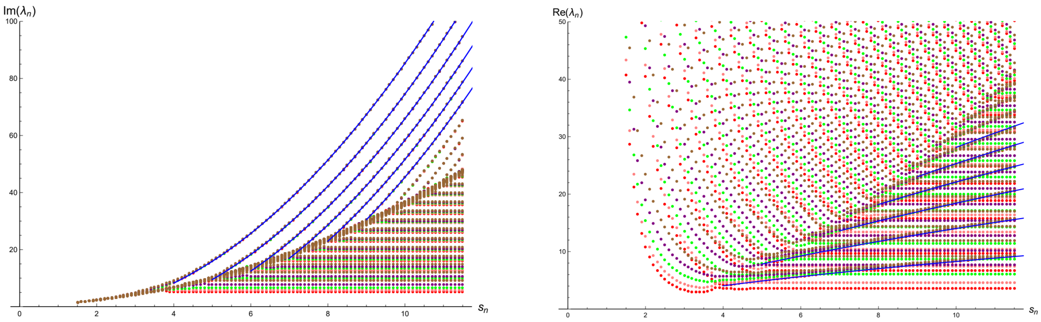

Figure 4.4: $V(x) = \mathrm{i}|x|^2$: Real (left) and imaginary (right) part of the eigenvalues of truncated operators $T_{n,l}$ with $d = 3$ and $l = 1, \ldots, 5$ (red, pink, green, purple, brown), defined on $L^2((1, s_n))$ with $s_n = 0.1n$, $n = 15, 16, \ldots, 115$. Asymptotic curves (blue) for $\lambda_{k,n}$ with the first correction for $k = 1, 2, \ldots, 6$.

Summary

In this thesis we studied spectral properties of Schrödinger operators. An overview of quantum mechanics with quasi-self-adjoint and non-self-adjoint operators was presented. Particularly the consistent interpretation of quantum mechanics in the case of quasi-self-adjoint observables was discussed and the crucial issue of noncompatibility of several quasi-self-adjoint observables was demonstrated

The most significant result is represented by explicit asymptotic formulae for eigenvalues derived and proven in three main settings. First, the linear and quadratic approximation of self-adjoint operators in Section 1.2, second, operators with strong coupling of imaginary part of the potential in enhanced dissipation and $\mathcal{PT}$-symmetric phase transition in Section 3.4 and last description of diverging eigenvalues occurring in domain truncation of Schrödinger operators with complex potentials in Chapter 4.

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Appendix: Publications Connected with Thesis

1. Znojil, M. and Semorádová, I. *Quantum square well with logarithmic central spike* Mod. Phys. Lett. A 33 (2018) 1850009

2. Znojil, M. and Semorádová, I.. *Log-anharmonic oscillator and its large-N solution* Mod. Phys. Lett. A 33.38 (2018) 1850223

3. Bagchi, B., Kamil. S.M., Tummuru, T.R., Semorádová, I., Znojil, M. *Branched Hamiltonians for a class of Velocity Dependent Potentials* Journal of Physics: Conference Series 839 (2017) 01201

4. Znojil, M., Semorádová, I., Růžička, F., Moulla, H., Leghrib, I. *The problem of coexistence of several non-Hermitian observables in PT-symmetric quantum mechanics* Phys. Rev. A 95 (2017) 042122 (2017)

5. Semorádová, I. and Siegl, P. *Diverging eigenvalues in domain truncations of Schrödinger operators with complex potentials* arXiv preprint arXiv:2107.10557