Czech Technical University in Prague
Faculty of Nuclear Sciences and Physical Engineering

**BACHELOR THESIS**

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# The concept of hidden hermicity and quantum graphs

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Název práce: **Koncept skryté hermitovosti a kvantové grafy**

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Abstrakt: Prozkoumáme se konceptem skryté hermitovosti, způsobem reprezentace kvantových pozorovatelných pomocí nesamosdružených operátorů. Zavedeme několik modelů majících vlastnost skryté hermitovosti, přičemž důraz bude kladen na přesnou řešitelnost a uplatnění v kvantové teorii katastrof. Zobecníme některé diferenciální operátory z jednoduchého intervalu na obecný kvantový graf a vyšetříme důsledky tohoto zobecnění. Spektrální vlastnosti všech zmíněných operatátorů budeme ilustrovat graficky pomocí pseudospekter.

Klíčová slova: skrytá hermitovost, kvantové katastrofy, kvantové grafy, pseudospektrum

Title: **The concept of hidden hermicity and quantum graphs**

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Abstract: We deal with the concept of crypto-self-adjointness, a way of representing quantum observables by non-self-adjoint operators. We examine a number of crypto-self-adjoint models of discrete and differential nature with emplasis on their exact solvability and application in the field of quantum catastrophes. We extend several differential models from a real interval to quantum graphs and examine the consequences. We illustrate properties of such models with the help of pseudospectra.

Keywords: hidden hermicity, quantum catastrophes, quantum graphs, pseudospectrum

# List of symbols

| | | |
|---|---|---|
| $\mathcal{H}$ | ... | separable Hilbert space |
| $\mathcal{L}(\mathcal{H})$ | ... | set of linear operators on $\mathcal{H}$ |
| $\mathcal{C}(\mathcal{H})$ | ... | set of closed operators on $\mathcal{H}$ |
| $\mathcal{B}(\mathcal{H})$ | ... | algebra of bounded operators on $\mathcal{H}$ |
| $\mathbf{H}$ | ... | linear operator |
| $\mathfrak{D}(\mathbf{H})$ | ... | domain of $\mathbf{H}$ |
| $\mathfrak{D}_{max}$ | ... | maximal domain of $\mathbf{H}$ |
| $\sigma(\mathbf{H})$ | ... | spectrum of $\mathbf{H}$ |
| $\sigma_\varepsilon(\mathbf{H})$ | ... | $\varepsilon$-pseudospectrum of $\mathbf{H}$ |
| $\mathbf{\Theta}$ | ... | metric operator |
| $\mathbf{\Omega}$ | ... | bounded similarity operator |
| $W^{k,l}$ | ... | Sobolev space |
| $\Delta$ | ... | Laplacian |
| $\mathfrak{D}_{obs}(\mathbf{H})$ | ... | domain of observability of $\mathbf{H}(\lambda)$ |
| $\|\psi\rangle$ | ... | Dirac ket |
| $\langle\psi\|$ | ... | Dirac bra |
| $\langle\langle\psi\|$ | ... | modified bra $\langle\psi\|\mathbf{\Theta}$ |
| $\mathbb{T}$ | ... | unit circle |
| $\mathbb{T}_n$ | ... | set of n-th roots of unity |
| $\leftrightarrow$ | ... | Wigner-Weyl correspondence |
| $\star$ | ... | phase-space star product |
| $\mathcal{G}$ | ... | quantum graph |
| $\mathcal{E}(\mathcal{G})$ | ... | set of edges of $\mathcal{G}$ |
| $\mathcal{V}(\mathcal{G})$ | ... | set of vertices of $\mathcal{G}$ |
| $\mathbb{W}$ | ... | positive-definite matrix |
| $\mathcal{P}$ | ... | operator of parity |
| $\mathcal{T}$ | ... | operator of time-reversal |
| $\mathcal{C}$ | ... | operator of charge |

# Contents


**Prologue** **2**

**1 Non-self-adjoint operators** **3**
- 1.1 Physics of non-self-adjoint operators . . . 3
- 1.2 The concept of crypto-self-adjointness . . . 5
- 1.3 Crypto-self-adjointness and quantum catastrophes . . . 7

**2 Discrete models** **9**
- 2.1 Theoretical aspects . . . 9
  - 2.1.1 Pseudospectrum . . . 9
- 2.2 Models . . . 10
  - 2.2.1 I: Discrete anharmonic oscillator . . . 11
  - 2.2.2 II: Chain model . . . 12
  - 2.2.3 III: Orthogonal polynomials . . . 13

**3 Differential models** **16**
- 3.1 Theoretical aspects . . . 16
  - 3.1.1 Quasi-exact solvability . . . 16
  - 3.1.2 Dieudonné equation in phase space . . . 17
  - 3.1.3 Klein-Gordon equation in quantum mechanics . . . 18
- 3.2 Models . . . 19
  - 3.2.1 I: Convection-diffusion operator . . . 19
  - 3.2.2 II: Complex Robin boundary conditions . . . 20
  - 3.2.3 III: Klein-Gordon model . . . 21

**4 Crypto-self-adjoint quantum graphs** **22**
- 4.1 Theoretical aspects . . . 22
  - 4.1.1 Graph Laplacian . . . 22
- 4.2 Models . . . 24
  - 4.2.1 I: Weighted/gauged Laplacian . . . 25
  - 4.2.2 II: Complex Robin boundary conditions . . . 26

**Conclusion** **28**

**Appendix** **29**
- A Rigged Hilbert spaces . . . 29
- B Spectral properties of crypto-self-adjoint operators . . . 30
- C Crypto-self-adjointness and antilinear symmetries . . . 31
- D Sectorial forms and operators . . . 31

# Prologue

The theory of self-adjoint operators on Hilbert spaces forms one of the central parts of mathematical physics [1, 2]. Motivated, above all, by ubiquitous presence of such operators in quantum physics [3], there exists vast literature on the topic, which may be perceived as well-understood.

The theory of non-self-adjoint (more generally non-normal) operators [4, 5] is much less developed. Attempts to carry over techniques from self-adjoint theory have limited success, although numerical experiments indicate the occurrence many new and unexpected phenomena [6]. A thorough understanding of non-self-adjoint operators is highly desirable, as they have a great importance in almost every area of physics: they are generally used to describe phenomena involving non-conservation of energy, like friction or drag forces. For a non-exhaustive list of examples, consider the Fokker-Planck equation in statistical physics [7], Black–Scholes equation in financial mathematics [8], Navier-Stokes equations in fluid dynamics [9], or nonlinear Schrödinger equation in optics [10]. In quantum mechanics, non-self-adjoint operators usually describe open quantum systems [11] or resonant phenomena [12].

Yet another promising application of non-self-adjoint operators emerged around 1992 in nuclear physics [13], where complicated bosonic operators were shown to admit a much simpler representation in terms of non-self-adjoint partners with identical spectral properties. Such operators were initially given the name *quasi-hermitian*: in the present work, they are called *crypto-self-adjoint*, following the terminology of [14]. This framework was later rediscovered in 1998 [15], when certain non-self-adjoint operators were shown to possess purely real spectrum, which was attributed to the $\mathcal{PT}$-symmetry of such operators [16]. The success of $\mathcal{PT}$-symmetric quantum mechanics led to a rapid progress in the field and may now be perceived as well-understood. This serves as a main motivation for the current task to use the crypto-self-adjoint framework in the case of quantum graphs.

Quantum graph theory is a well-established field of physics [17], which has its roots in direct phenomenology: quantum graphs are used to model atomic bonds in quantum chemistry [18], waveguides in quantum computing [19], carbon nanotubes in the study of graphene [20] or photonic crystals [21] in optics. They found applications also in the study of quantum chaos [22], scattering theory [23], theory of dynamical systems [24], the Hall effect [25] or Anderson localization [26]. Recent attempts to study quantum graph models in the crypto-self-adjoint framework include [27] and [28], which are also among the main inspirations for the present work.

This thesis aims to provide a compact review of the current state of art of regarding crypto-self-adjoint models and their applications. Moreover, it attempts to generalize some of the known differential models by promoting them from real line to a general quantum graph. It is divided into four chapters: chapter 1 motivates the study of non-self-adjoint operators in physics with the help of illustrative examples, and introduces the central concept of crypto-self-adjointness. Chapters 2 to 4 deal respectively with a number of discrete/differential/graph models. Necessary theoretical concepts needed to study the models are presented at the beginning of each chapter. Problems of mathematical nature are finally elaborated in the appendices.

# Chapter 1

# Non-self-adjoint operators

## 1.1 Physics of non-self-adjoint operators

Much of the success of spectral theory in analysis of self-adjoint (more generally normal) operators may be attributed to the *spectral theorem* [3], which establishes equivalence between normal and unitarily diagonalizable operators. More precisely, for any $\mathbf{H} \in \mathcal{C}(\mathcal{H})$ normal, there exists an unitary map $\mathbf{U} : \mathcal{H} \to L^2(\mathbb{R}), \quad f \in L^2(\mathbb{R})$, such that

$$[\mathbf{UHU}^{\dagger}\psi](x) = f(x)\psi(x) \qquad \forall \psi \in L^2(\mathbb{R}) \tag{1.1}$$

This means that up to an unitary transformation, the knowledge of spectrum of a normal operator is equivalent to the knowledge of the operator itself. This is not the case for non-normal operators.

In this introductory section, we aim to show that the predictions based on the spectrum itself may turn out to be misleading or plainly wrong, when dealing with non-normal operators. Generally, we shall be dealing with first order equations of the form $\dot{x} = \mathbf{H}x$ or $\mathrm{i}\dot{x} = \mathbf{H}x$, leading to the study of semigroups $\exp(t\mathbf{H})$ or $\exp(\mathrm{i}t\mathbf{H})$. While the spectrum can be employed to understand behavior of these semigroups as $t \to \infty$, their behavior over the entire range of $t$ is controlled by the resolvent norm of $\mathbf{H}$ [29]. In the case of non-normal operators, this can be a wildly behaving quantity (2.2). To illustrate such phenomena, we consider two examples from various fields of classical physics.

**Example (Orr-Sommerfeld operator) [6]**

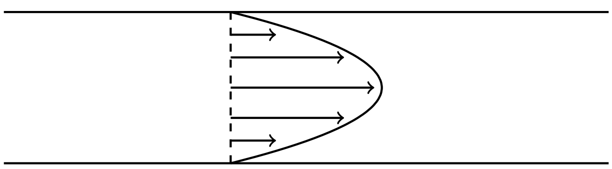

Figure I: Laminar flow in an infinite tube

One of the most famous phenomena showing manifest non-normality is turbulence in fluid mechanics. Consider a fluid described by incompressible Navier-Stokes equations [9] in an infinitely long 2D tube of fig. I. We know that in the 2D case, the Navies-Stokes equations admit smooth solution for any boundary conditions. However, the stability of such a solution is much more delicate issue. We make the ansatz

$$\psi(x, y, t) = u(x, t)\exp(\mathrm{i}\alpha y) \qquad \alpha > 0 \qquad u(\pm 1) = u_x(\pm 1) = 0 \tag{1.2}$$

and insert it into the Navier-Stokes equations. This results into a single equation $\dot{x} = \mathbf{H}x$ with

$$\mathbf{H} = \mathrm{i}\alpha\left(\frac{d^2}{dx^2} - \alpha^2\right)^{-1}\left[\frac{1}{\mathrm{i}\alpha R}\left(\frac{d^2}{dx^2} - \alpha^2\right)^2 - (1 - x^2)\left(\frac{d^2}{dx^2} - \alpha^2\right) - 2\right] \tag{1.3}$$

with $R$ being the Rayleigh quotient. This non-normal operator is called *Orr-Sommerfeld operator*. It can be shown, for $R$ small enough, to possess discrete spectrum contained in the left half of the complex plane [30], which means the corresponding solution decays do zero as $t \to \infty$. In fig. II one can see the eigenvalues and pseudospectra of (1.3): in all pseudospectral plots, the axes denote the real and imaginary parts of $\lambda$. Strong penetration of pseudospectra (2.1) into the right half-plane indicates the presence of a big jump of $\|\exp(t\mathbf{H})\|$ before decaying to zero, which is indeed related to the presence of turbulence.

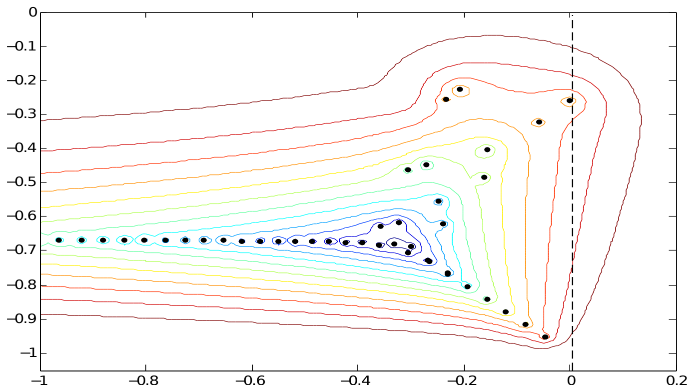


Figure II: Pseudospectra (2.1) of the Orr-Sommerfeld operator

**Example (Optical resonators) [6]**

Another problem of non-normal nature is ubiquitous in the theory of lasers. A laser beam building setup usually consists of two mirrors placed around the gain medium that form a standing wave cavity resonator for light waves. This problem is inherently non-normal since the mirror at one end of the cavity must reflect imperfectly, so that some light can escape from the cavity.

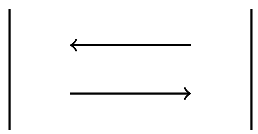

Figure III: Laser beam generating setup

The dynamics is governed by free-field Maxwell equations, which can be equivalently expressed as the electric field wave equation $E_{xx} + E_{yy} + k^2 E = 0$. The ansatz of solution propagating in the $y$-direction,$E(x,y) = \exp(-\mathrm{i}ky)u(x,y)$, leads to a reduced equation $u_{xx} + u_{yy} - 2\mathrm{i}ku_y = 0$. We use standart *paraxial approximation* and assume $u_{yy} \ll 1$, which reduces the equation to

$$u_y = -\frac{\mathrm{i}}{2k} u_{xx} \tag{1.4}$$

The solutions of this equation are not in $L^2(\mathbb{R})$ and have to be regularized using Fourier transform. This results in

$$u(x,y) = \mathbf{H}u_0(x,0) = \sqrt{\frac{\mathrm{i}k}{2\pi y}} \int_{\mathbb{R}} \exp\left(-\frac{\mathrm{i}k(x-t)^2}{2y}\right) u(t,0)dt \tag{1.5}$$

with $\mathbf{H}$ being a normal (unitary) integral operator. Let's now truncate this general unitary operator to the setting of fig. III. A two-dimensional cavity of length L is open at sides and bounded at the ends with two mirrors, located as $x = \pm 1$. Consequently, (1.5) reduces to a non-normal operator

$$u(x) = \mathbf{H}u_0(x) = \sqrt{\frac{\mathrm{i}k}{2\pi L}} \int_{-1}^{1} \exp\left(-\frac{\mathrm{i}k(x-t)^2}{2L}\right) u_0(t)dt \tag{1.6}$$

with the graphical analysis again using pseudospectra (2.1) shown in fig. IV.

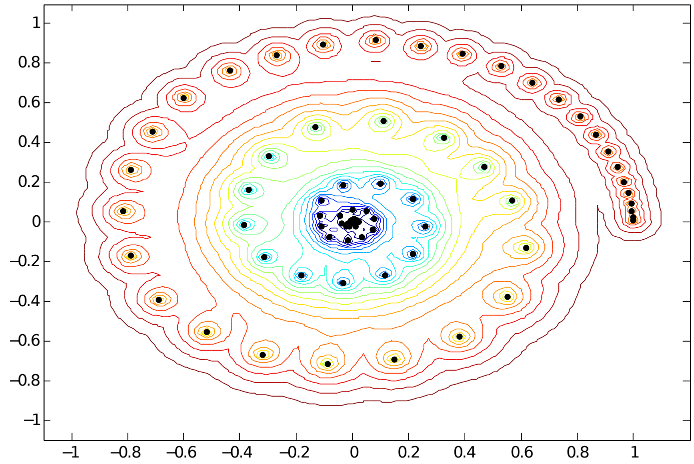


Figure IV: Pseudospectra of the of integral operator (1.6)

## 1.2 The concept of crypto-self-adjointness

Following the ideas of [13], let us elaborate on the possiblity of actual quantum *observables* being represented by non-self-adjoint operators. Consider a quantum system described by a Hilbert space $\mathcal{H}$ and a set of observables $\mathbf{H} \in \mathcal{C}(\mathcal{H})$. Then the observables are required to be self-adjoint by standard postulates of quantum mechanics. Their spectrum has to be real, because it corresponds to physically measurable quantities. Their eigenvectors have to form an orthonormal basis of $\mathcal{H}$, which follows from the projection postulate. Any operator having such properties is necessarily self-adjoint in $\mathcal{H}$. For operators with $\mathfrak{D}(\mathbf{H}) = \mathfrak{D}(\mathbf{H}^\dagger)$, we may write, using Dirac bra-ket notation

$$\mathbf{H}^\dagger = \sum_n |\psi_n\rangle\langle\psi_n|\mathbf{H}^\dagger = \sum_n \lambda_n^* |\psi_n\rangle\langle\psi_n| = \sum_n \lambda_n |\psi_n\rangle\langle\psi_n| = \mathbf{H}\sum_n |\psi_n\rangle\langle\psi_n| = \mathbf{H} \tag{1.7}$$

Note, however, that our choice of the representation of the physical Hilbert space, which we shall denote $\mathcal{H}^{(F)}$, is specified by formal rather than physical considerations. Although the action of a given observable $\mathbf{H}$ fixes the vector space, there is still freedom in choice of inner product. Some operators non-self-adjoint on $\mathcal{H}^{(F)}$ may become self-adjoint, and thus eligible as quantum observables, merely by changing the Hilbert space from $\mathcal{H}^{(F)}$ to $\mathcal{H}^{(S)}$, which differs in the choice of inner product. We may express the inner products in terms of *metric operators* $\mathbf{\Theta}$ as

$$\langle\phi|\psi\rangle_\Theta = \langle\phi|\mathbf{\Theta}|\psi\rangle \tag{1.8}$$

The self-adjointness of quantum observable $\mathbf{H} \in \mathcal{C}(\mathcal{H})$ in $\mathcal{H}^{(S)}$ can be expressed as

$$\langle\phi|\mathbf{\Theta}\mathbf{H}\psi\rangle = \langle\phi|\mathbf{H}\psi\rangle_\Theta = \langle\mathbf{H}\phi|\psi\rangle_\Theta = \langle\mathbf{H}\phi|\mathbf{\Theta}\psi\rangle = \langle\phi|\mathbf{H}^\dagger\mathbf{\Theta}\psi\rangle \tag{1.9}$$

Operators having such property shall be called *crypto-self-adjoint*. Equation (1.9) may be rewritten as

$$\mathbf{H}^\dagger\mathbf{\Theta} = \mathbf{\Theta}\mathbf{H} \tag{1.10}$$

and shall be referred to as *Dieudonné equation* [31].

| Hilbert space | ket | bra | inner product |
|---|---|---|---|
| $\mathcal{H}^{(F)}$ (unphysical) | $\|\psi\rangle$ | $\langle\psi\|$ | $\langle\psi\|\psi\rangle$ |
| $\mathcal{H}^{(S)}$ (physical) | $\|\psi\rangle$ | $\langle\langle\psi\| = \langle\psi\|\mathbf{\Theta}$ | $\langle\langle\psi\|\psi\rangle = \langle\psi\|\mathbf{\Theta}\|\psi\rangle$ |
| $\mathcal{H}^{(T)}$ (physical) | $\mathbf{\Omega}\|\psi\rangle$ | $\langle\psi\|\mathbf{\Omega}^\dagger$ | $\langle\psi\|\mathbf{\Omega}^\dagger\mathbf{\Omega}\|\psi\rangle = \langle\psi\|\mathbf{\Theta}\|\psi\rangle$ |

Table I: Three Hilbert spaces used in crypto-self-adjoint framework [32]

Solving the Dieudonné equation for a variety of models is the central part of this work. If $\mathbf{H}$ is self-adjoint in the classical sense, then $\mathbf{\Theta} = \mathbf{I}$ is a solution of (1.10). Moreover, it we assume $\mathbf{\Theta}$ to admit a decomposition

$\boldsymbol{\Theta} = \boldsymbol{\Omega}^\dagger \boldsymbol{\Omega}$ with $\boldsymbol{\Omega}$ invertible, we can show $\mathbf{H}$ to be similar to a self-adjoint operator $\mathbf{h}$ as

$$\mathbf{h} = \boldsymbol{\Omega}\mathbf{H}\boldsymbol{\Omega}^{-1} = \left(\boldsymbol{\Omega}\mathbf{H}\boldsymbol{\Omega}^{-1}\right)^\dagger = \mathbf{h}^\dagger \tag{1.11}$$

It is clear that $\mathbf{H}$ and $\mathbf{h}$ are isospectral as long as $\boldsymbol{\Omega}$ is bounded. For such $\boldsymbol{\Omega}$, it follows that $\boldsymbol{\Theta}$ is also bounded and boundedly invertible. We therefore restrict attention to metric operators satisfying the conditions of boundedness and bounded invertibility. In the language of spectral theorem (1.1), we have broadened the class of operators with real spectrum eligible as quantum observables from unitarily diagonalizable to boundedly diagonalizable ones, or from those with orthonormal basis of eigenvectors to those with Riesz basis of eigenvectors (B.2). The operator $\mathbf{h}$ acts in yet another Hilbert space representation, which shall be denoted $\mathcal{H}^{(T)}$, and may be assumed complicated.

Whenever we know $\boldsymbol{\Omega}$ explicitly, there is no reason to work with $\mathbf{H}$, as we can just as well work with its self-adjoint partner (1.11). However, as pointed out in [13], $\mathbf{h}$ may be in general a very complicated operator, whereas $\mathbf{H}$ would have a simple solvable form. This makes crypto-self-adjoint framework a great model-building scheme, in which one starts with a simple non-self-adjoint operator with real spectrum, and then examines its possible similarity to a much more complicated self-adjoint observable.

**Example**

For a simple illustrative example, consider $\mathcal{H}^{(F)} = \mathbb{R}^2$ with standard inner product and standard basis, and the operator $\mathbf{H}$ acting as

$$\mathbf{H} = \begin{bmatrix} 1 & 1 \\ 0 & 2 \end{bmatrix} \tag{1.12}$$

This matrix, despite being non-hermitian, is diagonalizable with real spectrum. By (B.2), this suffices to establish the crypto-self-adjointness of $\mathbf{H}$. Nevertheless, we shall construct the operators $\boldsymbol{\Theta}$ and $\boldsymbol{\Omega}$ explicitly. The Dieudonné equation (1.10) has the form

$$\begin{bmatrix} 1 & 0 \\ 1 & 2 \end{bmatrix} \boldsymbol{\Theta} = \boldsymbol{\Theta} \begin{bmatrix} 1 & 1 \\ 0 & 2 \end{bmatrix} \tag{1.13}$$

and its solution can be written explicitly in a two-parametric form

$$\boldsymbol{\Theta} = \begin{bmatrix} a & -a \\ -a & b \end{bmatrix} \qquad b > a > 0 \tag{1.14}$$

Yet another way to calculate $\boldsymbol{\Theta}$ is to compute the eigenkets of $\mathbf{H}$ and insert them in the spectral resolution series (**??**). This yields the expression

$$\boldsymbol{\Theta} = \sum_{n=1}^{2} |\phi_n\rangle\langle\phi_n| = a \begin{bmatrix} -1 \\ 1 \end{bmatrix} \begin{bmatrix} -1 & 1 \end{bmatrix} + b \begin{bmatrix} 0 \\ 1 \end{bmatrix} \begin{bmatrix} 0 & 1 \end{bmatrix} = \begin{bmatrix} a & -a \\ -a & a+b \end{bmatrix} \qquad a, b > 0 \tag{1.15}$$

which indeed agrees with (1.13). We proceed to compute the operator $\boldsymbol{\Omega} = \boldsymbol{\Theta}^{1/2}$. We choose $\boldsymbol{\Omega}$ to be a mapping $\mathbb{R}^2 \to \mathbb{R}^2$ for simplicity. One of its solutions is

$$\boldsymbol{\Theta} = \boldsymbol{\Omega}^\dagger \boldsymbol{\Omega} = \begin{bmatrix} \sqrt{a(1-a/b)} & -a/\sqrt{b} \\ 0 & \sqrt{b} \end{bmatrix} \begin{bmatrix} \sqrt{a(1-a/b)} & 0 \\ -a/\sqrt{b} & \sqrt{b} \end{bmatrix} \tag{1.16}$$

and the self-adjoint partner $\mathbf{h}$ of $\mathbf{H}$ is given by

$$\boldsymbol{\Omega}\mathbf{H}\boldsymbol{\Omega}^{-1} = \begin{bmatrix} 1/\sqrt{a(1-a/b)} & 1/\sqrt{b(1-a/b)} \\ 0 & 1/\sqrt{b} \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 0 & 2 \end{bmatrix} \begin{bmatrix} \sqrt{a(1-a/b)} & -a/\sqrt{b} \\ 0 & \sqrt{b} \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 2 \end{bmatrix} \tag{1.17}$$

and we see that the off-diagonal element can be indeed transformed away by a similarity transform. The properties of the respective spaces are summarized in table II.

| Hilbert space | vector space | inner product | basis |
|---|---|---|---|
| $\mathcal{H}^{(F)}$ | $\mathbb{C}^2$ | $\begin{bmatrix}\phi_1 & \phi_2\end{bmatrix}\begin{bmatrix}\psi_1\\ \psi_2\end{bmatrix}$ | $(\begin{bmatrix}1\\0\end{bmatrix},\begin{bmatrix}0\\1\end{bmatrix})$ |
| $\mathcal{H}^{(S)}$ | $\mathbb{C}^2$ | $\begin{bmatrix}\phi_1 & \phi_2\end{bmatrix}\begin{bmatrix}a & -a\\ -a & b\end{bmatrix}\begin{bmatrix}\psi_1\\ \psi_2\end{bmatrix}$ | $(\begin{bmatrix}1\\0\end{bmatrix},\begin{bmatrix}0\\1\end{bmatrix})$ |
| $\mathcal{H}^{(T)}$ | $\mathbb{C}^2$ | $\begin{bmatrix}\phi_1 & \phi_2\end{bmatrix}\begin{bmatrix}\psi_1\\ \psi_2\end{bmatrix}$ | $(\mathbf{\Omega}\begin{bmatrix}1\\0\end{bmatrix},\mathbf{\Omega}\begin{bmatrix}0\\1\end{bmatrix})$ |

Table II: Three-Hilbert-space framework apllied to the model (1.12)

## 1.3 Crypto-self-adjointness and quantum catastrophes

Studying crypto-self-adjoint operators in $\mathcal{H}^{(F)}$ does, in addition to a simplification of mathematics, lead to yet another interesting phenomena. One such phenomenon emerges when we let $\mathbf{H}$ to depend on (one or more) parameters $\lambda$. We assume that the dependence on $\lambda$ is analytic and that $\mathbf{H}(\lambda)$ is crypto-self-adjoint for at least one $\lambda \in \mathbb{R}$ and denote

$$\mathfrak{D}_{obs}(\mathbf{H}) = \{\, \lambda \in \mathbb{R} \mid \mathbf{H}(\lambda) \text{ is crypto-self-adjoint } \} \tag{1.18}$$

The analytic dependence on $\lambda$ results in the fact, that (1.10) holds for any $\lambda \in \mathbb{R}$, although the positivity of $\mathbf{\Theta}$ may not be satisfied. In the light of (C), this shows that the spectrum of $\mathbf{H}(\lambda)$ outside $\mathfrak{D}_{obs}(\mathbf{H})$ remains invariant with respect to complex conjugation. Therefore, complexification of spectrum is anticipated by pairwise coalescence of $\lambda \in \sigma(\mathbf{H})$. Moreover, from (C) follows also, that even the eigenvectors merge at $\mathfrak{D}_{obs}(\mathbf{H})$, making the operator nondiagonalizable at the boundary of observability.

Such points are classic examples of *exceptional points*, introduced by Kato in the context of perturbation theory [4], whose physical importance has been emphasized in ionised state physics [33], resonance phenomena [34], chirality [35] or microwave cavities [36]. We see that in crypto-self-adjoint quantum mechanics, exceptional points describe loss of observability of $\mathbf{H}(\lambda)$ in $\mathcal{H}^{(F)}$. Note that exceptional points may occur also in the case of self-adjoint operators for (unphysical) complex parameter values, which is usually manifested by a phenomenon of avoided crossings, see fig. V. As illustrative example, consider a simple hermitian and crypto-hermitian matrices

$$\begin{aligned}
\mathbf{H} &= \begin{bmatrix}1 & \lambda\\ \lambda & -1\end{bmatrix} \qquad |\psi\rangle = \begin{bmatrix}\lambda/(\sqrt{1-\lambda^2}-1)\\ 1\end{bmatrix}, \begin{bmatrix}-\lambda/(\sqrt{1-\lambda^2}+1)\\ 1\end{bmatrix} \qquad \lambda_{EP} = \pm\mathrm{i}\\
\mathbf{H} &= \begin{bmatrix}1 & \lambda\\ -\lambda & -1\end{bmatrix} \qquad |\psi\rangle = \begin{bmatrix}\lambda/(\sqrt{1-\lambda^2}-1)\\ 1\end{bmatrix}, \begin{bmatrix}-\lambda/(\sqrt{1-\lambda^2}+1)\\ 1\end{bmatrix} \qquad \lambda_{EP} = \pm 1
\end{aligned} \tag{1.19}$$

The phenonenon of observability loss at certain $\lambda \in \mathbb{R}$ shall be called *quantum catastrophe* [37]. This name is not accidental, as it describes phenomena of great qualitative changes caused by small perturbations in operator theory, just as classical theory of catastrophes [38] does it in function theory.

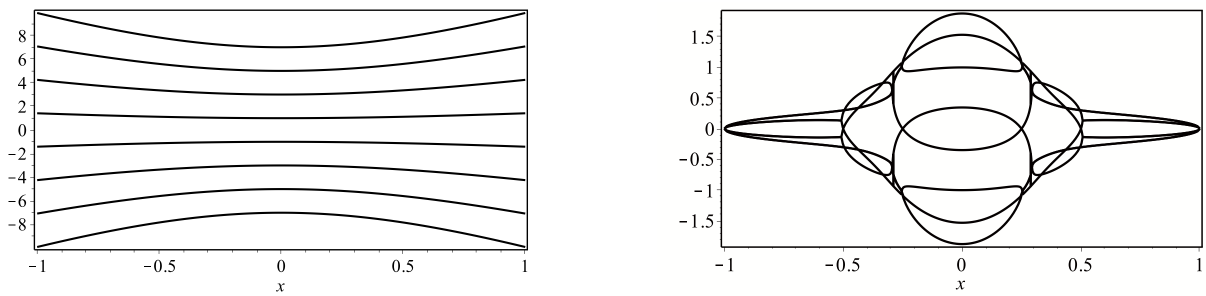


Figure V: Generic behavior of eigenvalues, self-adjoint and crypto-self-adjoint case

**Example [39]**

Consider a harmonic oscillator on $L^2(\mathbb{R})$, regularized in the sense that $x \to x - \mathrm{i}c$, resulting in

$$\mathbf{H} = -\frac{d^2}{dx^2} + x^2 - 2\mathrm{i}cx + \frac{\alpha^2 - 1/4}{(x - \mathrm{i}c)^2} \qquad \mathfrak{D}(\mathbf{H}) = \mathfrak{D}_{max} \tag{1.20}$$

the spectrum of such operator is remains purely discrete and available in explicit form as

$$E_{n\pm} = 4n + 2 \pm 2\alpha + c^2 \tag{1.21}$$

which is manifestly real, degenerate for $\alpha \in \mathbb{Z}$ and nondegenerate otherwise. It has been proven in [39] that the operator is indeed nondiagonalizable $\alpha \in \mathbb{Z}$, thus having genuine exceptional points at these parameter values.

# Chapter 2

# Discrete models

## 2.1 Theoretical aspects

### 2.1.1 Pseudospectrum

The concept of $\varepsilon$-pseudospectum of a non-normal operator [6] is an invaluable tool for both analytical and numerical study of non-normal operators, which has been proven already in fig. II and fig. IV. It is defined as a simple generalization of spectrum through analytical properties of resolvent function:

$$\sigma_\varepsilon(\mathbf{H}) = \left\{ \lambda \in \mathbb{C} \middle| \|(\mathbf{H} - \lambda)^{-1}\| \geq \varepsilon^{-1} \right\} \tag{2.1}$$

To understand the behavior of resolvent, we remind a classic inequality [4], valid for any $\mathbf{H} \in \mathcal{C}(\mathcal{H})$

$$\frac{1}{\rho\left[\lambda, \sigma(\mathbf{H})\right]} \leq \|(\mathbf{H} - \lambda)^{-1}\| \tag{2.2}$$

with $\rho(x, y)$ denoting the Euclidean metric. This inequality implies that the $\varepsilon$-neighborhood of spectrum is always the subset of $\varepsilon$-pseudospectrum. Moreover, a direct consequence of the spectral theorem (1.1) is the reverse inequality [6], making behavior of $\varepsilon$-pseudospectra trivial in the case of normal operators. When examining crypto-self-adjoint operators in $\mathcal{H}^{(F)}$, we can apply this result to its self-adjoint partner $\mathbf{h} = \mathbf{\Omega H \Omega^{-1}}$ to show, that the resolvent of $\mathbf{H}$ satisfies the inequalities

$$\frac{1}{\rho\left[\lambda, \sigma(\mathbf{H})\right]} \leq \|(\mathbf{H} - \lambda)^{-1}\| \leq \frac{\|\mathbf{\Omega}\| \|\mathbf{\Omega^{-1}}\|}{\rho\left[\lambda, \sigma(\mathbf{H})\right]} \tag{2.3}$$

We can conclude that for a crypto-self-adjoint $\mathbf{H}$ with bounded but highly non-unitary $\mathbf{\Omega}$, the pseudospectrum can form very non-trivial patterns, similar to those of fig. II and fig. IV.

**Example (pseudospectra of Toeplitz matrices)**

Pseudospectra of non-normal operators often reveal patterns invisible from the spectrum itself. This is illustrated in case of *Toeplitz matrices* [40], matrices constant along diagonals. A special case of a Toeplitz matrix is a *circulant matrix* with $a_{k-n} = a_k$. Every circulant matrix is normal, while most Toeplitz non-circulant matrices are not [41].

$$\mathbf{H_n^{(T)}} = \begin{bmatrix} a_0 & a_1 & & \dots & a_{n-1} \\ a_{-1} & a_0 & & & \vdots \\ & \ddots & \ddots & \ddots & \\ \vdots & & & a_0 & a_1 \\ a_{1-n} & \dots & & a_{-1} & a_0 \end{bmatrix} \qquad \mathbf{H_n^{(c)}} = \begin{bmatrix} a_0 & a_1 & & \dots & a_{n-1} \\ a_{n-1} & a_0 & & & \vdots \\ & \ddots & \ddots & \ddots & \\ \vdots & & & a_0 & a_{-1} \\ a_1 & \dots & & a_{n-1} & a_0 \end{bmatrix} \tag{2.4}$$

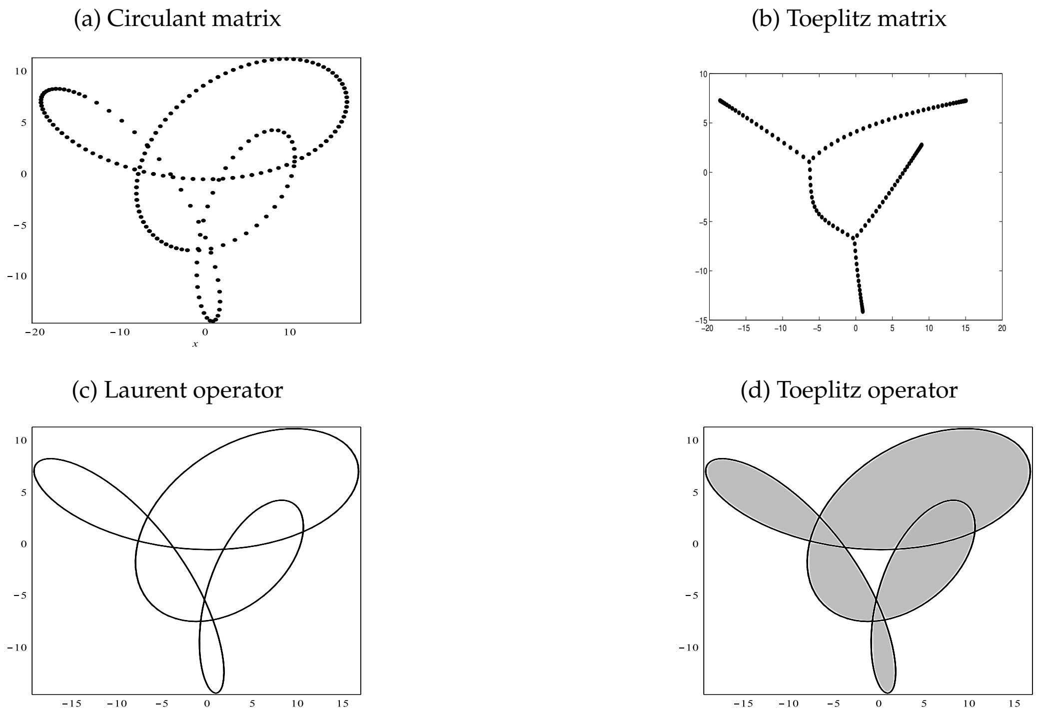


Figure VI: Spectra of operator associated with (2.6), $n = 150$ for matrices

We shall be interested also in infinite-dimensional analogues of Toeplitz and circulant matrices. They are called, respectively, *Toeplitz operators* and *Laurent operators*. Here we restrict attention to bounded operators of such kind, which enables us to define a meromorphic complex function

$$f(z) = \sum a_k z^k \tag{2.5}$$

For $f(z)$ having no singularities on the unit circle, the spectra of general Toeplitz operators, as well as those of circulant matrices, admit a simple characterization in terms of $f(z)$ [6]. Let $\mathbb{T}$ denote the unit circle and $\mathbb{T}_n$ the set of n-th roots of unity.

- For a circulant matrix $\mathbf{H_n}$, we have $\sigma(\mathbf{H_n}) = f(\mathbb{T}_n)$.
- For a Laurent opeator $\mathbf{H}$ , we have $\sigma(\mathbf{H}) = f(\mathbb{T})$.
- For a Toeplitz operator $\mathbf{H}$, we have $\sigma(\mathbf{H}) = f(\mathbb{T})$ together with its interior.

To illustrate the statements of this theorem, fig. VI shows the spectra of all considered operators associated with the symbol

$$f(z) = \frac{\mathrm{i}}{2z^3} - \frac{5}{z^2} + \frac{6}{z} - 3z^2 - 8\mathrm{i}z^3 \tag{2.6}$$

As a direct corollary of the above statements, the $\ell^2$-convergence of a sequence of circulant matrices implies the convergence of spectra (in the Hausdorff metric). From fig. VI, it is also obvious that it does not hold for a convergent sequence of general Toeplitz matrices. In this case, the look at the pseudospectra of such a sequence proves very illuminating, as illustrated in fig. VII. The figures suggest the result that can be indeed proven rigorously [42] about the convergence of $\varepsilon$-pseudospectra:

$$\|\mathbf{H_n} - \mathbf{H}\|_{\ell^2} \to 0 \Longrightarrow \sigma_\varepsilon(\mathbf{H_n}) \to \sigma_\varepsilon(\mathbf{H}) \tag{2.7}$$

## 2.2 Models

We present a number of discrete crypto-self-adjoint models, which appear naturally in the study of spin or the Klein-Gordon (3.12) and Proca [43] equations. Another motivation shall be seen in the final chapter, where the

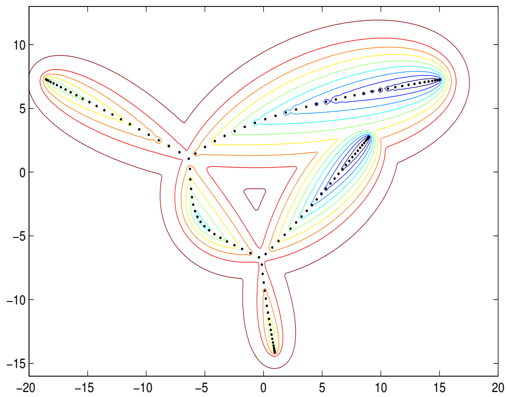


Figure VII: Pseudospectra of the Toeplitz matrix associated with (2.6)

Laplacian $\Delta$ on quantum graph $\mathcal{G}$ shows to be of to an extent reducible to the matrix of its boundary conditions (4.4). Our principal motivation for studying such systems originates from the concept of quantum catastrophes (1.18), which proves much more feasible in the matrix framework. Finite-dimensional quantum-catastrophes are even already classified [44] in parallel to the classification of elementary catastrophes in classical theory [38].

### 2.2.1 I: Discrete anharmonic oscillator

This model, studied in [45], can be regarded as an equidistant Runge-Kutta [46] discretization of the imaginary anharmonic oscillator [15]

$$\mathbf{H} = -\frac{d^2}{dx^2} + x^2(\mathrm{i}x)^\varepsilon \qquad \mathfrak{D}(\mathbf{H}) = \mathfrak{D}_{max} \tag{2.8}$$

This oscillator can be shown to possess a real spectrum [47], but the fact that all of its metric operators are inherently unbounded or singular [48], makes it fall out of the scope of the present work. On the other hand, its discretized counterpart admits genuine quantum-mechanical interpretation. It is sampled for dimension 6 as

$$\mathbf{H_6} = \begin{bmatrix} \gamma i & 1 & & & & \\ 1 & \beta i & 1 & & & \\ & 1 & \alpha i & 1 & & \\ & & 1 & -\alpha i & 1 & \\ & & & 1 & -\beta i & 1 \\ & & & & 1 & -\gamma i \end{bmatrix} \tag{2.9}$$

Quantum catastrophes motivate the study of exceptional points occuring generically at $\mathfrak{D}_{obs}$ (C). In general, this procedure involves calculating all eigenvalues of $\mathbf{H}$ and finding the domain of their simultaneous positivity. We use, however, a simpler method method of calculating $\mathfrak{D}_{obs}$ for low matrix dimensions $2n$ without need to explicitly calculate the eigenvalues [49]. The secular equation of a general $2n \times 2n$ matrix model reads

$$\lambda^{2n} - P_{(n-1)}\lambda^{2n-1} + P_{(n-2)}\lambda^{2n-2} - ... + P_0 = 0 \tag{2.10}$$

From the invariance of eigenvalues with respect to complex conjugation even outside $\mathfrak{D}_{obs}(\mathbf{H})$ (C), and rescaling the coefficients $P_k$ conveniently, we might recast (2.10) into the form

$$s^n - \binom{n}{1}P_{(n-1)}s^{n-1} + \binom{n}{2}P_{(n-2)}s^{n-2} - ... + \binom{n}{n}P_0 = 0 \qquad s = \lambda^2 \tag{2.11}$$

where the condition $\lambda \in \mathbb{R}$ becomes $s \geq 0$. The coefficients $P_k$ can be expressed by well-known formulas in

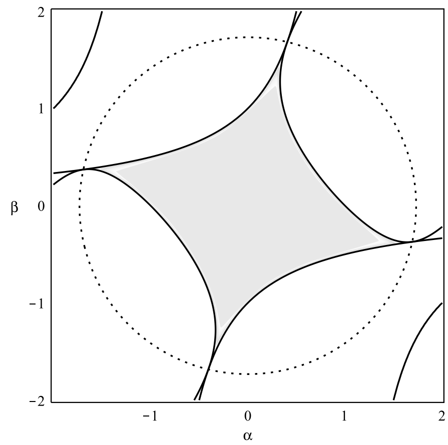


Figure VIII: Domains of observability of (2.9) for $\mathbf{H_4}$

terms of polynomial roots, resulting in a simple necessary condition for the reality of spectrum

$$\begin{aligned} s_1 + s_2 + ... + s_n &= P_{(n-1)} \geq 0 \\ s_1 s_2 + s_1 s_3 + ... + s_{n-1} s_n &= P_{(n-2)} \geq 0 \\ s_1 s_2 s_3 + s_1 s_2 s_4 + ... + s_{n-2} s_{n-1} s_n &= P_{(n-3)} \geq 0 \end{aligned} \tag{2.12}$$

For $n \leq 11$, we are able to reverse the statement, and give a sufficient condition for $s \geq 0$ from the coefficients $P_k$ themselves, which means we are able to express $\mathfrak{D}_{obs}$ exactly up to a polynomial of order 22! The complete list is given in [49], we write explicitly the simples case of $n = 2, 3$.

$$\begin{aligned} n = 2: &\quad P_1, P_2 \geq 0, &\quad P_1^2 \geq P_2 \\ n = 3: &\quad P_1, P_2, P_3 \geq 0, &\quad 3P_1^2 P_2^2 + 6P_1 P_2 P_3 \geq 4P_2^3 + P_3^2 + 4P_3 P_1^3 \end{aligned} \tag{2.13}$$

The domain of observability of (2.9) is sampled in fig. VIII for $n = 2$. The cusp shape of $\mathfrak{D}_{obs}$ seems to be characteristic for oscillator models and relevant to cusp catastrophes in classical catastrophe theory [38].

### 2.2.2 II: Chain model

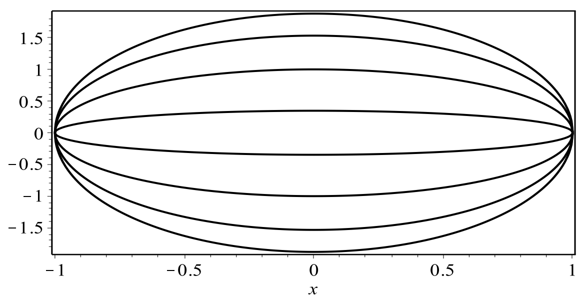


Figure IX: Big banging spectrum of model (2.16) for $n = 8$

This model [50] may be seen as inspired by the harmonic oscillator Hamiltonian in energy representation, complemented with a (sufficiently small) antisymmetric perturbation. It is again made dependent on $n$ general parameters, which can be expressed sampled for dimension 6 as

$$\mathbf{H_6} = \begin{bmatrix} -5 & \gamma & & & & \\ -\gamma & -3 & \beta & & & \\ & -\beta & -1 & \alpha & & \\ & & -\alpha & 1 & \beta & \\ & & & -\beta & 3 & \gamma \\ & & & & -\gamma & 5 \end{bmatrix} \tag{2.14}$$

The general recipe (2.13) may be employed in unchanged manner to construct $\mathfrak{D}_{obs}(\mathbf{H})$. Exceptional symmetry of $\mathfrak{D}_{obs}(\mathbf{H})$, as seen in fig. X, served as a motivation in [50] to search for the cusp locations in closed form. Extensive use of symbolic manipulations has provided a conjecture, that the coordinates of maximally degenerate EPs of model (2.14) are given by

$$g_n^{(EEP)} = \sqrt{n(N-n)}, \quad n = 1, ..., N \tag{2.15}$$

which can be verified simply by insertion. This enables us to achieve interesting maximal degeneracy scenarios, sampled in fig. IX, by a simple tuning of parameters. Such maximal degeneracy of eigenvalues has been shown relevant e.g. in [51] the context of cosmology. The fine-tuned matrix is sampled for dimension 4 as

$$\mathbf{H_4^{(BB)}} = \begin{bmatrix} -3 & \sqrt{3}\lambda & & \\ -\sqrt{3}\lambda & -1 & 2\lambda & \\ & -2\lambda & 1 & \sqrt{3}\lambda \\ & & -\sqrt{3}\lambda & 3 \end{bmatrix} \tag{2.16}$$

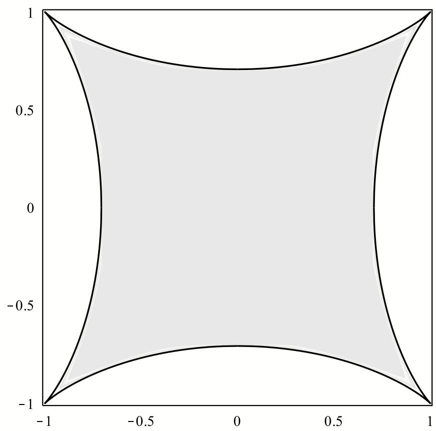


Figure X: Domains of observability of (2.14) for $\mathbf{H_4}$

### 2.2.3 III: Orthogonal polynomials

This model exploits the well-known correspondence between orthogonal polynomials [52] and tridiagonal matrices to establish a broad family of crypto-hermitian models. We say, that a polynomial sequence $(P_n)_{n=0}^{\infty}$ is *orthogonal*, if there exists a measure $\mu$ on $\mathbb{R}$, such that

$$\langle P_m | P_n \rangle = \int_{\mathbb{R}} P_m(x) P_n(x) d\mu(x) = 0 \quad \text{for} \quad m \neq n \tag{2.17}$$

We list two relevant results from the theory of orthogonal polynomials, which can be found in [52]. Let $P_n(x)$ be an orthogonal polynomial sequence.

$$\begin{aligned} &\bullet \quad \text{It obeys } xP_n(x) = a_n P_{n+1}(x) + b_n P_n(x) + c_n P_{n-1}(x) \text{ for } b_n \in \mathbb{R}, a_n c_n > 0 \\ &\bullet \quad \text{Every } P_n(x) \text{ has } n \text{ distrinct real roots.} \end{aligned} \tag{2.18}$$

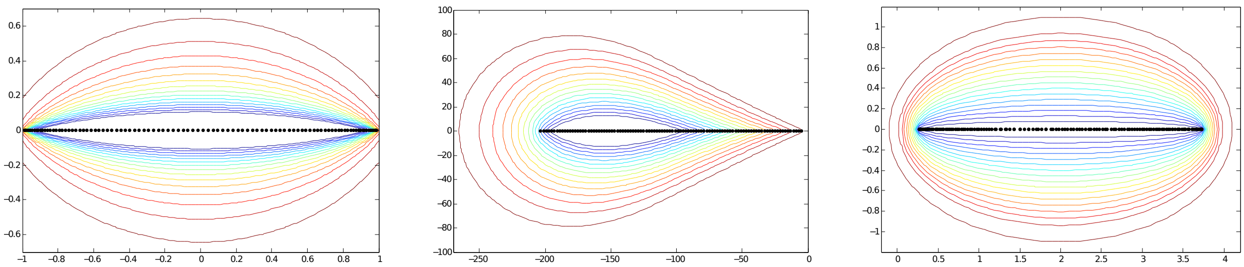

Figure XI: Pseudospectra of OPS of Gegenbauer-type, Laguerre-type and the example (2.23) for $n = 100$

Orthogonal polynomials admit a simple representation in terms of tridiagonal matrices. To see this, it suffices to observe that the sequence of characteristic polynomials of

$$\mathbf{H_n} = \begin{bmatrix} b_1 & a_1 & 0 & \dots & 0 & 0 \\ c_2 & b_2 & a_2 & \dots & 0 & 0 \\ 0 & c_3 & b_3 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & b_{n-1} & a_{n-1} \\ 0 & 0 & 0 & \dots & c_n & b_n \end{bmatrix} \tag{2.19}$$

satisfies the recurrence (2.18), and thus defines an orthogonal polynomial sequence. The $n-th$ member of the series has $n$ real nondegenerate roots, which proves its crypto-hermicity. Curiously enough, this family of matrices admits a general solution of the Dieudonné equation in a recurrent form [53]. Consider the equation $\mathbf{H_n^\dagger \Theta_n} = \mathbf{\Theta_n H_n}$, with (2.19) reparametrized as

$$\mathbf{H_n} = \begin{bmatrix} a_{11} & a_{12} & 0 & \dots & 0 \\ a_{21} & a_{22} & a_{23} & \dots & 0 \\ 0 & a_{23} & a_{33} & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & 0 & \dots & a_{nn} \end{bmatrix} \qquad \mathbf{\Theta_n} = \begin{bmatrix} \theta_{11} & \theta_{12} & \theta_{13} & \dots & \theta_{1n} \\ \theta_{12}^* & \theta_{22} & \theta_{23} & \dots & \theta_{2n} \\ \theta_{13}^* & \theta_{23}^* & \theta_{33} & \dots & \theta_{3n} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ \theta_{1n}^* & \theta_{2n}^* & \theta_{3n}^* & \dots & \theta_{nn} \end{bmatrix} \tag{2.20}$$

Comparing both sides of Dieudonné equation elementwise elementwise yields $\theta_{ij} = \theta_{ij}^*$ and a set of recurrences for the (real) matrix elements $\theta_{ij}$

$$\begin{aligned} a_{(k+1)k}\theta_{(k+1)(k+n-1)} &= a_{k(k+1)}\theta_{k(k+n)} \\ b_k\theta_{k(k+n-1)} + c_{k+1}\theta_{(k+1)(k+n)} &= a_{k+2}\theta_{k(k+n-1)} + b_k\theta_{(k)(k+n-1)} \\ &\dots \\ &\dots \\ \textstyle\sum_{j=1}^n a_{(n+k)n}\theta_{(n+k)(n+1)} &= \textstyle\sum_{j=1}^n a_{(n+k+1)(n+1)}\theta_{(n)(n+k+1)} \end{aligned} \tag{2.21}$$

These recurrences, when solved from the first one downwards, admit explicit solution, with $n$ free parameters $\theta_{11}, ..., \theta_{1n}$ admitting to be chosen along the way. As a special case, when assuming a diagonal metric ansatz in (2.20), the recurrences degenerate into

$$\theta_{j+1} = \theta_j \frac{a_j}{c_{j+1}} \tag{2.22}$$

**Example [54]**

Motivated again by the problem of quantum catastrophes (1.18), we construct a family of $n$-parametric $2n \times 2n$ matrices, shown for dimension 6

$$\mathbf{H_6} = \begin{bmatrix} 0 & 1-\gamma & & & & \\ 1+\gamma & 0 & 1-\beta & & & \\ & 1+\beta & 0 & 1-\alpha & & \\ & & 1+\alpha & 0 & 1-\beta & \\ & & & 1+\beta & 0 & 1-\gamma \\ & & & & 1+\gamma & 0 \end{bmatrix} \tag{2.23}$$

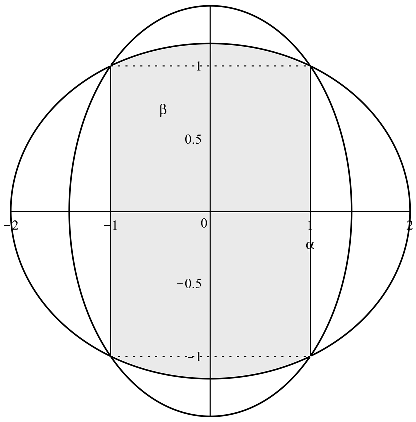


Figure XII: Domains of observability of (2.23) for $\mathbf{H_4}$

Such matrices obey the three term recurrence (2.18) for $\alpha, \beta, \gamma, ... \in (-1, 1)$. This would suggest that the domain of observability is a mere hypercube in the multiparametric space, which is further supported by contructing a simplest diagonal metric operator from the recurrences (2.22), whose domain of positivity is precisely that hypercube.

Curiously enough, plotting of the actual domain of observability of fig. XII shows $\mathfrak{D}_{obs}(\mathbf{H})$ larger than conjectured. This means, that despite the singularity of the metric and breakdown of the orthogonal polynomial framework, there exist some (non-diagonal) metric operators positive for a larger domain of parameters. This model can again be simply tuned to show the big-baning spectrum of (2.16): it suffices to fix

$$\alpha = \beta = \gamma = ... = \lambda \tag{2.24}$$

# Chapter 3

# Differential models

## 3.1 Theoretical aspects

### 3.1.1 Quasi-exact solvability

Exactly solvable models lie in the center of quantum mechanics. Besides their direct application to phenomenology, they serve as a starting point for perturbative approximations, and admit observation of non-perturbative effects themselves [55]. However, currently known exactly solvable models form a limited family: they are basically just the harmonic oscillator, the hydrogen-like atom, Morse potential, Pöschl-Teller potential and a few others [56]. This motivates a generalization of the concept of exact solvability, which would broaden the range of operators while preserving most of its above-mentioned merits. Such generalization is found in the concept of quasi-exact solvability [57].

We say that a self-adjoint operator $\mathbf{H}$ is *exactly solvable*, if its eigenvalue equation can be transformed into hypergeometric equation by a change of variables. That means we are able to construct a basis of hypergeometric functions $(\psi_n)$, such that it diagonalizes the operator

$$(\mathbf{H}_{ij}) = \left(\langle\psi_i|\mathbf{H}|\psi_j\rangle\right) = \operatorname{diag}\,(\lambda_i) \tag{3.1}$$

understood again in the sense of (A). Similarly, we call a self-adjoint operator $\mathbf{H}$ *quasi-exactly solvable*, if some basis of hypergeometric functions $(\psi_n)$ transforms it into

$$(\mathbf{H}_{ij}) = \left[\begin{array}{ccc|c} H_{11} & \dots & H_{1n} & \\ \vdots & \ddots & \vdots & \\ H_{n1} & \dots & H_{nn} & \\ \hline & & & \text{nonzero elements} \end{array}\right] \tag{3.2}$$

In such case, the upper left block of $\mathbf{H}$ is finite and its diagonalization is an algebraic process. A finite number of eigenvalues can be expressed as polynomial roots, and the corresponding eigenvectors remain in elementary form. The concepts of exact and quasi-exact solvability can be naturally generalized to crypto-self-adjoint models, with the notion of orthonormal basis replaced by Riesz basis (B.2).

#### Example (sextic oscillator)

Generalizations of harmonic oscillator are natural potentials to examine when searching for quasi-exactly solvable models. We shall see shortly that the quartic oscillator does not enjoy such a property, making the sextic oscillator, studied in [58], a next-to-trivial choice. It is defined on $L^2(\mathbb{R})$ as

$$\mathbf{H} = -\frac{d^2}{dx^2} + ax^2 + bx^4 + cx^6 \qquad \mathfrak{D}(\mathbf{H}) = \mathfrak{D}_{max} \tag{3.3}$$

where we shall assume $c > 0$, so that $V(x)$ is an infinite potential well with a purely discrete spectrum in the light of [59]. Inspired by the eigenfunctions of harmonic oscillator, we formulate wavefunction ansatz

$$\psi(x) = \exp\left(-\frac{\alpha x^2}{2} - \frac{\beta x^4}{4}\right) \sum_{n=0}^{\infty} \xi_n x^{2n} \tag{3.4}$$

is insert it into $\mathbf{H}\psi(x) = \lambda\psi(x)$. Comparing coefficients of such a polynomial series pairwisely yields a five-term recurrence relation $a_n\xi_{n+2} + b_n\xi_{n+1} + c_n\xi_n + d_n\xi_{n-1} + e_n\xi_{n-2} = 0$ with

$$\begin{aligned} a_n &= -2n(2n+1) \qquad & c_n &= a + 3\beta + 2\beta n - \alpha^2 \qquad & e_n &= c - \beta^2 \\ b_n &= \alpha + 2\alpha n - \lambda \qquad & d_n &= b - 2\alpha\beta \end{aligned} \tag{3.5}$$

We can refine the wavefunction ansatz (3.4) by the choice $\alpha = b/2\sqrt{c},\ \beta = \sqrt{c}$, which makes (3.5) degenerate into a three-term recurrence with

$$a_n = -(2n+1)(2n) \qquad b_n = \frac{b}{2\sqrt{c}} + \frac{bn}{\sqrt{c}} - \lambda \qquad c_n = 3\sqrt{c} - \frac{b^2}{4c} + 2\sqrt{c}n + a \tag{3.6}$$

correspoding to a tridiagonal infinite matrix $(\mathbf{H}_{ij}) = \langle\psi_i|\mathbf{H}|\psi_j\rangle$. In order to achieve the block-diagonal form (3.2), we need one of the elements $a_n, c_n$ to vanish for some $n \in \mathbb{N}$. The only option here is $c_n = 0$, resulting in

$$\frac{1}{\sqrt{c}}\left(\frac{b^2}{4c} - a\right) = 2n + 3 \qquad n \in \mathbb{N} \tag{3.7}$$

As long as this constraint is satisfied, (3.3) is quasi-exactly solvable and $(\mathbf{H}_{ij})$ is a block-diagonal matrix with a finite $n \times n$ block. Note that when $c = 0$ (the quartic oscillator [55]), the model is not quasi-exactly solvable for *any* values of $a, b$.

### 3.1.2 Dieudonné equation in phase space

Solving the Dieudonné equation (1.10) in infinite-dimensional spaces can be often very difficult of even impossible. An alternative approach can be applied for operators on $L^2(\mathbb{R}^n)$ using techniques of phase-space quantum mechanics [60], in particular the Wigner-Weyl transform [61]. The Wigner-Weyl transform is a bijection $\leftrightarrow$ between closed operators on $L^2(\mathbb{R}^n)$ and smooth functions on $\mathbb{R}^n$, which can be shown [61] to have the following properties:

(3.8)

- $\mathbf{x} \leftrightarrow x, \quad \mathbf{p} \leftrightarrow p$
- $\mathbf{H}$ bounded $\leftrightarrow H(x,p)$ bounded
- $\mathbf{H} \leftrightarrow H(x,p)$ if and only if $\mathbf{H}^\dagger \leftrightarrow H^*(x,p)$
- $\mathbf{H} \geq 0 \leftrightarrow H(x,p) \geq 0$

In the phase space, the role of non-commutative operator multiplication is played by the *star product*, a mapping compatible with the Wigner-Weyl transform in the sense that

$$\star : \mathbb{R}^n \times \mathbb{R}^n \longrightarrow \mathbb{R}^n \qquad \mathbf{F} \cdot \mathbf{G} \leftrightarrow F(x,p) \star G(x,p) \tag{3.9}$$

The most commonly used form of star product is the *Moyal product* [62], defined as

$$\begin{aligned} F(x,p) \star G(x,p) &= F(x,p) \exp\left(\frac{1}{2}(\overleftarrow{\partial_x}\overrightarrow{\partial_p} - \overleftarrow{\partial_p}\overrightarrow{\partial_x})\right) G(x,p) \\ &= \sum_{n=0}^{\infty}\sum_{k=0}^{n} \frac{(-i)^n(-1)^k}{2^n n!}\binom{n}{k} \frac{\partial^n F(x,p)}{\partial x^k \partial p^{n-k}} \frac{\partial^n G(x,p)}{\partial p^k \partial x^{n-k}} \end{aligned} \tag{3.10}$$

With this knowledge in mind, we are able to transform the operator Dieudonné equation into its phase-space equivalent, a partial differential equation. We compute a phase-space counterpart of $\mathbf{H} \leftrightarrow H(x,p)$ and solve the equation

$$H^*(x,p) \star \Theta(x,p) = \Theta(x,p) \star H(x,p) \tag{3.11}$$

for $\Theta$ satisfying $\varepsilon \leq \Theta(x,p) \leq K$. Note that this PDE has finite order only if $H(x,p)$ is a polynomial in $x$ and $p$, which is a often encountered but not ubiquitous phenomenon.

### 3.1.3 Klein-Gordon equation in quantum mechanics

The Klein-Gordon equation [59] is one of the relativistic versions of the Schrödinger equation. It is a basic equation in quantum electrodynamics, where it describes time evolution of a charged spinless scalar field. In a free-field form, it reads

$$\left(\Box + \frac{m^2c^2}{\hbar^2}\right)\psi(x,t) = 0 \tag{3.12}$$

The original purpose of the Klein-Gordon equation was to describe relativistic spinless particles in quantum mechanic. Such approach however encountered a fundamental obstacle regarding negative probability densities, and had to be abandoned for almost 80 years. In this section, following the ideas of [63], we make quantum-mechanical interpretation of the Klein-Gordon equation possible, using tools of crypto-self-adjoint quantum mechanics.

Postulates of quantum mechanics make each solution of the Schrödinger equation $|\psi(t)\rangle \in \mathcal{H}$ generate a probability density $\rho(x,t)$: a function which is non-negative, integrable and locally conserved, meaning that it obeys the continuity equation $\rho_t + \nabla\vec{j} = 0$ for some $\vec{j}$. This could be satisfied by the choice

$$\rho(x,t) = |\psi(x,t)|^2 = |\langle x|\psi(t)\rangle|^2 \qquad \vec{j}(x,t) = \frac{i\hbar}{2m}(\psi^*\nabla\psi - \psi\nabla\psi^*) \tag{3.13}$$

Equivalently, this means that $\rho(x,t)$ corresponds to an inner product conserved in time

$$\langle\phi(t)|\psi(t)\rangle = \int_{\mathbb{R}} \rho(x,t)dx = \int_{\mathbb{R}} |\psi(x,t)|^2 dx \tag{3.14}$$

To make the Klein-Gordon equation a genuine part of quantum mechanics, it is necessary to find relativistic analogues of (3.13) and (3.14). Intuition would suggest to replace (3.13) by a four-current

$$j^\mu(x,t) = \frac{i\hbar}{2m}(\psi^*\partial^\mu\psi - \psi\partial^\mu\psi^*) \tag{3.15}$$

which can be shown to be indeed locally conserved with a correct $c \to \infty$ limit [**?** ]. However, the null component of $j^\mu$, aiming to describe the probability density, does not satisfy the positivity condition. Equivalently, the corresponding *Klein-Gordon inner product* is indefinite.

$$\rho = \frac{1}{c}j^0 = \frac{i\hbar}{2mc^2}\left(\psi^*\frac{\partial\psi}{\partial t} - \frac{\partial\psi^*}{\partial t}\psi\right) \qquad \langle\phi|\psi\rangle_{KG} = \frac{i\hbar}{2mc^2}\left(\langle\phi|\dot{\psi}\rangle - \langle\dot{\phi}|\psi\rangle\right) \tag{3.16}$$

which necessitates the current (3.15) to be abandoned as non-physical. In further search for physically correct quantitites, we make use of crypto-self-adjoint theory. We rewrite the equation (3.12) as

$$\ddot{\psi}(x,t) + \mathbf{D}\psi(x,t) = 0 \qquad \mathbf{D} = -\Delta + \frac{m^2c^2}{\hbar^2} \tag{3.17}$$

which can be recast into a system of two first-order PDEs in the so-called Feschbach-Villars representation [64].

$$i\hbar\dot{\Psi}(x,t) = \mathbf{H}\Psi(x,t) \qquad \Psi(t) = \begin{bmatrix} i\dot{\psi}(x,t) \\ \psi(x,t) \end{bmatrix} \qquad \mathbf{H} = \hbar\begin{bmatrix} 0 & \mathbf{D} \\ \mathbf{I} & 0 \end{bmatrix} \tag{3.18}$$

As long as $\mathbf{D} = \mathbf{D}^\dagger$ in $L^2(\mathbb{R})$, we may conjecture that $\mathbf{H}$ is crypto-self-adjoint in $L^2(\mathbb{R}) \bigoplus L^2(\mathbb{R})$, and construct metric operators by summing the spectral resolution series (B.8).

$$\mathbf{\Theta} = \alpha_+\begin{bmatrix} 1 & -\mathbf{D}^{1/2} \\ -\mathbf{D}^{1/2} & \mathbf{D} \end{bmatrix} + \alpha_-\begin{bmatrix} 1 & \mathbf{D}^{1/2} \\ \mathbf{D}^{1/2} & \mathbf{D} \end{bmatrix} = (\alpha_+ + \alpha_-)\begin{bmatrix} 1 & \frac{\alpha_- - \alpha_+}{\alpha_+ + \alpha_-}\mathbf{D}^{1/2} \\ \frac{\alpha_- - \alpha_+}{\alpha_+ + \alpha_-}\mathbf{D}^{1/2} & \mathbf{D} \end{bmatrix} \tag{3.19}$$

By denoting $\alpha = \frac{\alpha_- - \alpha_+}{\alpha_+ + \alpha_-}$ and neglecting global multiplication by a constant, we get

$$\mathbf{\Theta} = \begin{bmatrix} 1 & \alpha\mathbf{D^{1/2}} \\ \alpha\mathbf{D^{1/2}} & \mathbf{D} \end{bmatrix} \qquad \alpha \in (-1,1) \tag{3.20}$$

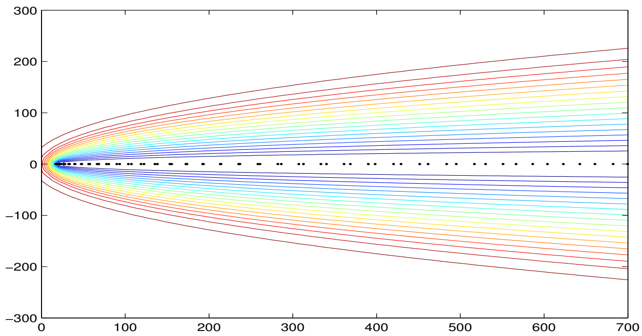


Figure XIII: spectrum and pseudospectra of (4.29) for $\mu = 0.015$ $(\kappa \sim 3.4 \times 10^{14})$

Such metric operators are apparently not bounded, which makes them fall out of the crypto-self-adjoint framework in the strict sense. It is however not the end of the story, as it is possible for the Dyson mapping $\mathbf{\Omega}$ to exist even in the case of unbounded metric operators [65]. The corresponding family of inner products is

$$\langle \phi|\psi\rangle_{\mathbf{\Theta}} = \langle \Phi|\mathbf{\Theta}|\Psi\rangle = \langle \phi|\mathbf{D}|\psi\rangle - \langle \dot{\phi}|\dot{\psi}\rangle + \mathrm{i}\alpha\left(\langle \phi|\mathbf{D^{1/2}}|\dot{\psi}\rangle - \langle \dot{\phi}|\mathbf{D^{1/2}}|\psi\rangle\right) \tag{3.21}$$

The explicit construction of the probability density $\rho(x,t)$ from $\langle \phi|\psi\rangle_{KG}$ is also possible, but shows to be more involved[63]. Note that the same procedure done here for the Klein-Gordon equation can be repeated for the Proca equation, as shown in [43].

## 3.2 Models

We introduce several differential operators defined on a finite interval instead of the whole $L^2(\mathbb{R})$. The reason for this is twofold: such models are readily generalized to the case of compact graphs, and also because the study of differential operators on $L^2(\mathbb{R})$ usually leads to unbounded or singular metric operators [48].

### 3.2.1 I: Convection-diffusion operator

This model takes inspiration from the phenomena of diffusion and convection, which appear very often in fluid dynamics, an obvious example being the Navier-Stokes equations. It was initially introduced in [6] and has the form

$$\mathbf{H_d} = -\mu\frac{d^2}{dx^2} + \frac{d}{dx} \qquad \mathfrak{D}(\mathbf{H_d}) = \{\, \psi \in W^{2,2}([0,d]) \,|\, \psi(0) = \psi(d) = 0 \,\} \tag{3.22}$$

The Dirichlet boundary conditions are chosen just for purposes of solvability: the procedure could be repeated for any boundary conditions of a self-adjoint Laplacian, see (4.8). In the Dirichlet case, the eigenvalue equation can be solved explicitly as

$$\lambda_n = -\frac{1}{4\mu} + \frac{\mu\pi^2 n^2}{d^2} \qquad \psi_n(x) = \exp\left(\frac{x}{2\mu}\right)\sin\left(\frac{\pi n}{d}x\right) = \exp\left(\frac{x}{2\mu}\right)\chi_n^D(x) \tag{3.23}$$

Because the eigenfunctions of the Dirichlet Laplacian $\chi_n^D(x)$ form a complete orthonormal basis, it is clear that $(\psi_n)$ is a Riesz basis (B.2) with $C = \max\{\,1, \exp(d/2\mu)\,\}$. This implies that (4.29) is crypto-self-adjoint and its spectrum is purely discrete. In this case, a similarity transformation $\mathbf{\Omega}$ can be guessed readily from the shape of eigenfunctions (3.23).

$$\mathbf{\Theta} = \exp\left(\frac{x}{\mu}\right) \qquad \mathbf{\Omega} = \mathbf{\Theta^{1/2}} = \exp\left(\frac{x}{2\mu}\right) \tag{3.24}$$

and the isospectral self-adjoint counterpart of $\mathbf{H_d}$ is

$$\mathbf{h_d} = \mathbf{\Omega}^{-1}\mathbf{H_d}\mathbf{\Omega} = -\mu\frac{d^2}{dx^2} + \frac{1}{4\mu^2} \qquad \mathfrak{D}(\mathbf{h_d}) = \mathfrak{D}(\mathbf{H_d}) \tag{3.25}$$

Such $\mathbf{\Theta}$ could be found also using the phase-space technique (3.11). The corresponding phase-space function yields $\mathbf{H} \leftrightarrow \mu p^2 + ip$, and the equation (3.11) reads

$$\Theta(x,p) = \mu \frac{\partial}{\partial x} \Theta(x,p) \tag{3.26}$$

The transformation $\mathbf{\Omega}$ is highly non-unitary for small $\mu$: its condition number is $\kappa = \|\mathbf{\Omega^{-1}}\|\|\mathbf{\Omega}\| = e^{1/2\mu}$. This is reflected in the non-trivial behavior of pseudospectra, shown in fig. XIII. In the limit $d \to \infty$, the metric operator becomes unbounded and $\mathbf{H}$ loses its crypto-self-adjointness property. Indeed, by Fourier transforming $\mathbf{H}$ on $L^2(\mathbb{R})$ into a multiplication operator $\mathbf{H} = \mu p^2 + ip$, we see that its spectrum forms a parabola in the complex plane:

$$\sigma(\mathbf{H}) = \{\, \lambda \in \mathbb{C} \;\big|\; \mathrm{Re}\,\lambda = (\mu\, \mathrm{Im}\,\lambda)^2 \,\} \tag{3.27}$$

which suggests, in parallel to (2.7), the convergence of pseudospectra of $\mathbf{H}_d$ to those of $\mathbf{H}$ in the limit $d \to \infty$.

### 3.2.2 II: Complex Robin boundary conditions

Boundary conditions of the Laplacian $\Delta$ admit a simple matrix characterization (4.4), with self-adjoint boundary conditions distinguished by a simple rule (4.8). It was suggested in [66] to turn attention to non-self-adjoint boundary conditions, whose spectral problem maintains the feature of explicit solvability. This is achieved in the case of

$$\Delta_\alpha = -\frac{d^2}{dx^2} \qquad \mathfrak{D}(\Delta_\alpha) = \{\, \psi \in W^{2,2}(-a,a) \;\big|\; \psi'(-a) = \mathrm{i}\alpha\psi(-a),\;\; \psi'(a) = \mathrm{i}\alpha\psi(a) \,\} \tag{3.28}$$

It can be directly verified that $\Delta_\alpha^\dagger = \Delta_{-\alpha}$, and the operator is non-self-adjoint for $\alpha \neq 0$. Solving its eigenvalue equation explicitly yields

$$\begin{aligned} \lambda_0 &= \alpha^2 & \psi_0^{(\alpha)}(x) &= \exp(\mathrm{i}\alpha(x+a)) \\ \lambda_n &= \frac{n^2\pi^2}{4a^2} & \psi_n^{(\alpha)}(x) &= \cos\left(\frac{\pi n}{2a}(x+a)\right) - \mathrm{i}\alpha\frac{2a}{\pi n}\sin\left(\frac{\pi n}{2a}(x+a)\right) \end{aligned} \tag{3.29}$$

which shows that the eigenvalues are real and $\psi_n^\alpha(x)$ are simple combinations of Dirichlet and Neumann eigenfunctions $\chi_n^N(x)$ and $\chi_n^D(x)$

$$\psi_n^\alpha(x) = \chi_n^N(x) - \mathrm{i}\alpha k_n \chi_n^D(x) \qquad \phi_n^\alpha(x) = \chi_n^N(x) + \mathrm{i}\alpha k_n \chi_n^D(x) \qquad k_n = \frac{2a}{\pi n} \tag{3.30}$$

which form orthonormal bases in $L^2([-a,a])$. This shows that $(\psi_n^\alpha)$ is a Riesz basis (B.2) of $L^2([-a,a])$ with $C = \max\{\,1, 1+2\alpha a/\pi\,\}$, and (3.28) is a crypto-self-adjoint operator. Moreover, the metric operator admits explicit construction by summing the spectral resolution series. Inserting (3.30) into (B.8) yields

$$\mathbf{\Theta}_\alpha = \sum_{n=0}^{\infty} |\phi_n^\alpha\rangle\langle\phi_n^\alpha| = \mathbf{I} - |\phi_0^\alpha\rangle\langle\phi_0^\alpha| - |\chi_0^N\rangle\langle\chi_0^N| + i\alpha\sum_{n=1}^{\infty}\frac{|\chi_n^D\rangle\langle\chi_n^N| - |\chi_n^N\rangle\langle\chi_n^D|}{k_n} + \sum_{n=1}^{\infty}\frac{|\chi_n^D\rangle\langle\chi_n^D|}{k_n^2} \tag{3.31}$$

Because $k_n^2$ are precisely the eigenvalues of the Dirichlet Laplacian, the last sum may be seen as a spectral resolution of inverse operator $(-\Delta_D)^{-1}$, which can be expressed in explicit integral form. Similarly, the middle sum is integrated by parts to yield

$$\mathrm{i}\sum_{n=1}^{\infty}\frac{|\chi_n^D\rangle\langle\chi_n^N| - |\chi_n^N\rangle\langle\chi_n^D|}{k_n} = \mathbf{p}\sum_{n=1}^{\infty}\frac{|\chi_n^D\rangle\langle\chi_n^D|}{k_n^2} + \mathbf{p}^*\sum_{n=1}^{\infty}\frac{|\chi_n^D\rangle\langle\chi_n^D|}{k_n^2} \tag{3.32}$$

with $\mathbf{p}$ and $\mathbf{p}^*$ being classical momentum operators with domains $W^{1,2}(-a,a)$, respectively $W_0^{1,2}(-a,a)$, yielding again the spectral resolutions for $(-\Delta_D)^{-1}$ and $(-\Delta_N)^{-1}$, with the latter understood in the sense of reduced resolvent [4]. Such operators admit expression in terms of integral kernel, which can be verified by direct multiplication. The kernels have the form

$$\mathcal{K}_D(x,y) = \frac{(x+a)(a-y)}{2a} \qquad \mathcal{K}_N(x,y) = \frac{(x+a)^2 + (y-a)^2}{4a} - \frac{a}{3} \qquad x < y \tag{3.33}$$

with the roles of $x, y$ reversed for $x > y$. Inserting formulas (3.32) and (3.33) into (3.31) yields the metric operator in a remarkably explicit form $\mathbf{\Theta} = \mathbf{I} + \mathbf{K}$, with the integral kernel of $\mathbf{K}$ being

$$\begin{aligned} \mathcal{K}(x,y) = \frac{\mathrm{i}}{a} \exp\left(\frac{\mathrm{i}\alpha}{2}(x-y)\right) \sin\left(\frac{\alpha}{2}(x-y)\right) - \\ -\frac{\mathrm{i}\alpha}{2a}(|x-y|-2a)\,\mathrm{sgn}(y-x) + \frac{\alpha^2}{2a}\left(a^2 - xy - a|y-x|\right) \qquad x>y \end{aligned} \tag{3.34}$$

We are even able to express the similarity operator $\mathbf{\Omega}$, as it can be directly verified that it admits an expression

$$\mathbf{\Omega} = |\chi_0^N\rangle\langle\phi_0| + \sum_{n=1}^{\infty} |\chi_n^N\rangle\langle\chi_n^N| - \mathrm{i}\alpha \sum_{n=1}^{\infty} \frac{|\chi_n^N\rangle\langle\chi_n^D|}{k_n} \tag{3.35}$$

which again admits integrating by parts into the form expressible by $(-\Delta_D)^{-1}$ and $(-\Delta_N)^{-1}$. The self-adjoint counterpart of (3.28) is then finally computed to be

$$\mathbf{h} = \mathbf{\Omega}\mathbf{H}\mathbf{\Omega}^{-1} = \Delta + \alpha^2|\chi_0^N\rangle\langle\chi_0^N| \qquad \mathfrak{D}(\mathbf{h}) = \{\,\psi \in W^{2,2} | \psi'(0) = \psi'(d) = 0\,\} \tag{3.36}$$

### 3.2.3 III: Klein-Gordon model

With the knowledge of the fresh quantum-mechanical interpretation of the Klein-Gordon equation (3.12), we illustrate solving such equation on a simple example. Using again the Feschbach-Villars representation of the Klein-Gordon equation

$$\begin{bmatrix} 0 & \mathbf{H} \\ \mathbf{I} & 0 \end{bmatrix} \begin{bmatrix} \phi(x) \\ \psi(x) \end{bmatrix} = \lambda \begin{bmatrix} \phi(x) \\ \psi(x) \end{bmatrix} \tag{3.37}$$

we see that the second row of (3.37) stands for $\phi(x) = \lambda\psi(x)$, and insertion into the first row results in $\mathbf{H}\psi = \lambda^2\psi$, thus making the eigenvalue Klein-Gordon equation reducible to a eigenvalue Schrödinger equation, with the eigenvalues having being related as

$$\lambda_{KG} = \pm\sqrt{\lambda_S} \tag{3.38}$$

We apply these results to the exactly solvable Pöschl-Teller potential [67]

$$\mathbf{H} = -\frac{d^2}{dx^2} - \frac{l(l+1)}{2\cosh^2(x)} \qquad \mathfrak{D}(\mathbf{H}) = \mathfrak{D}_{max} \tag{3.39}$$

which a finite well decaying to zero as $x \to \pm\infty$, suggesting [59] that is admits a finite number of bound states below continuous ionized spectrum. In search for the bound states, we use the wavefunction ansatz

$$\psi(x) = \sum_{n=0}^{\infty} \frac{\xi_n}{\cosh^{2n}(x)} \tag{3.40}$$

Inserting $\psi(x)$ into the Schrödinger equation, one gets a three-term recurrence formula

$$a_n = -(n-1)(n-2) \qquad b_n = 2n^2 - l(l+1) - \lambda \qquad c_n = l(l+1) - (n-2)(n-1) \tag{3.41}$$

To terminate such a recurrence, it is necessary that $\lambda \in \mathbb{N}$. The solution of the resulting finite-dimensional algebraic problem can be written in terms of Legendre polynomials as $\lambda_n = -n^2 \quad \psi_n(x) = P_\lambda^n(\tanh(x))$ for $n = 1, 2 \ldots l$. This yields the result for the Klein-Gordon eigenvalues

$$\lambda_n = n \qquad n = -l \ldots l \tag{3.42}$$

# Chapter 4

# Crypto-self-adjoint quantum graphs

## 4.1 Theoretical aspects

This section aims to apply the crypto-self-adjoint formalism to operators on *quantum graphs* [17], which are simply oriented graphs $\mathcal{G}$ [68] together with a Hilbert space $\mathcal{H}(\mathcal{G})$. Such Hilbert space is traditionally constructed, in parallel with the real line case, by we associating each edge $\varepsilon \in \mathcal{E}(\mathcal{G})$ to a length $a_\varepsilon \in \mathbb{R}_+$ and a measure $dx_\varepsilon$, and taking the space of square-integrable function with respect to such measure

$$\mathcal{H}(\mathcal{G}) = \bigoplus_\varepsilon \mathcal{H}_\varepsilon = \bigoplus_\varepsilon L^2([0, a_\varepsilon], dx_\varepsilon) \tag{4.1}$$

The inner product on $\mathcal{H}(\mathcal{G})$ shall be assumed, again in parallel with $L^2(\mathbb{R})$, to be

$$\langle \phi | \psi \rangle_\mathcal{G} = \sum_\varepsilon \langle \phi | \psi \rangle_\varepsilon = \sum_\varepsilon \int_\varepsilon \phi^*(x_\varepsilon) \psi(x_\varepsilon) dx_\varepsilon \tag{4.2}$$

### 4.1.1 Graph Laplacian

The Laplacian $\Delta$ acting on arbitrary quantum graph $\mathcal{G}$ with various boundary conditions imposed at the vertices is a well-motivated [69] and well-explored [70] subject. It turns out that many important properties of $\Delta$ follow already from the matrices of vertex boundary conditions. Here we review several possible ways to construct such matrices and characterize the boundary conditions [27], which are defined as extensions of a minimal Laplacian

$$\Delta_{min} = -\frac{d^2}{dx^2} \qquad \mathfrak{D}(\Delta_{min}) = \{ \psi \in W^{2,2}(\mathcal{G}) \mid \psi(v) = 0,\ \psi'(v) = 0 \ \ \forall v \in \mathcal{V} \} \tag{4.3}$$

For a graph $\mathcal{G}$ with a single vertex, we proceed in the following way: we construct a vector of boundary values $\psi(v) = [\psi_1(v), ..., \psi_{d_v}(v)]^T$ and introduce three possible $d_v$-dimensional matrix parametrizations

$$\begin{array}{lll} \bullet & \mathbb{A}\psi(v) + \mathbb{B}\psi'(v) = 0 & \text{general} \\ \bullet & ik(\mathbb{U} - \mathbb{I})\psi(v) + (\mathbb{U} + \mathbb{I})\psi'(v) = 0 & \text{regular} \\ \bullet & \mathbb{P}\psi(v) = 0, \quad \mathbb{Q}\psi'(v) + \mathbb{L}\mathbb{Q}\psi(v) = 0 & \text{sectorial} \end{array} \tag{4.4}$$

For a graph $\mathcal{G}$ with more that one vertex, we can always reduce it into a single-vertex graph, as illustrated in fig. XIV. Moreover, because we shall be working exclusively with *local* boundary conditions, we can always define $\psi(v) = (\psi(v_1), ..., \psi(v_n))^T$ and the global matrices of dimension $\sum d_v$ as

$$\mathbb{A}\psi(v) + \mathbb{B}\psi'(v) = 0 \qquad \mathbb{A} = \operatorname{diag}(\mathbb{A}_v) \qquad \mathbb{B} = \operatorname{diag}(\mathbb{B}_v) \tag{4.5}$$

The general parametrization apparently parametrizes all possible extensions of (4.3), whereas the other two parametrizations do not. The regular parametrization for a given $k$ can be obtained through the transformation

$$\mathbb{U}(k) = -(\mathbb{A} + ik\mathbb{B})^{-1}(\mathbb{A} - ik\mathbb{B}) \tag{4.6}$$

and the sectorial parametrization is found by taking $\mathbb{P}$ to be orthogonal pojection on ker $\mathbb{B}$, $\mathbb{Q}$ to be orthogonal projection of $(\text{ran}\mathbb{B})^{\perp}$, and

$$\mathbb{L} = (\mathbb{B}|_{\text{ran}\, B^{\dagger}})^{-1}\mathbb{A}\mathbb{P}^{\perp} \tag{4.7}$$

In the rest of this section, we provide a systematic characterization of extensions of $\Delta_{min}$. We shall always assume $\dim(\mathbb{A}, \mathbb{B}) = \sum d_v$, otherwise the operator can be shown to have a trivial spectrum [27].

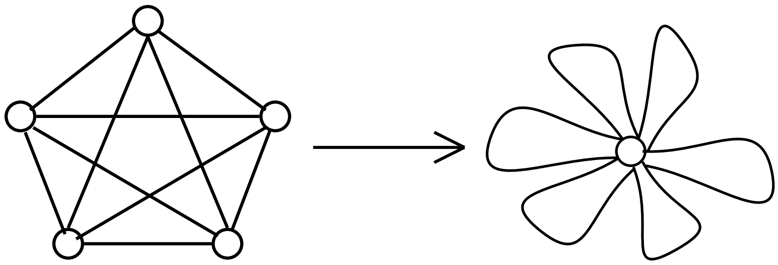

Figure XIV: Every compact graph $\mathcal{G}$ can be deformed to a single-vertex graph

### Self-adjoint boundary conditions

It is a simple excercise to verify that (4.3) is a symmetric operator with deficiency indices $(n, n)$, thus admitting a number of self-adjoint extensions. A classical result of Von Neumann's extension theory [3] states, that $\Delta$ is a self-adjoint operator if and only if admits the regular parametrization (4.4) with $k = 1$ and $\mathbb{U}$ unitary. Using the inverse to (4.6), which has the form

$$\mathbb{A} = \mathbb{I} - \mathbb{U} \qquad \mathbb{B} = \frac{\mathbb{I} + \mathbb{U}}{ik} \tag{4.8}$$

and the transformation (4.7), which will be shown to always exist in this case (4.11), we establish equally simple conditions of self-adjointness for regular and sectorial parametrizations [**?** ], with the results

$$\mathbb{A}\mathbb{B}^{\dagger} = \mathbb{B}\mathbb{A}^{\dagger} \qquad \mathbb{U}^{-1} = \mathbb{U}^{\dagger} \qquad \mathbb{L} = \mathbb{L}^{\dagger} \tag{4.9}$$

Example of self-adjoint conditions are the ordinary Robin boundary conditions with $\alpha, \beta \in \mathbb{R}$ and

$$\mathbb{A} = \begin{bmatrix} \alpha & 0 \\ 0 & \beta \end{bmatrix} \qquad \mathbb{B} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \tag{4.10}$$

### M-sectorial boundary conditions

Contrary to the general parametrization (4.4), regular and sectorial parametrizations to not describe all extensions of $\Delta_{min}$. They do, however, correspond to certain important classes of operator. Here we justify the name for the sectorial parametrization: it was shown in [71], that the operator $\mathbb{L}$ from (4.7) exists ($\mathbb{B}|_{\ker B^{\dagger}}$ is invertible) if and only if $\Delta$ is m-sectorial (D), and that it is equivalent to the condition

$$\mathbb{Q}\mathbb{A}\mathbb{P}^{\perp} = 0 \tag{4.11}$$

As an example of such boundary conditions, consider the conditions corresponding to complex $\delta$-interaction [17]

$$\mathbb{A} = \begin{bmatrix} 1 & -1 \\ \alpha & 0 \end{bmatrix} \qquad \mathbb{B} = \begin{bmatrix} 0 & 0 \\ 1 & 1 \end{bmatrix} \tag{4.12}$$

which are apparently not self-adjoint for $\alpha \notin \mathbb{R}$, whereas the criterion (4.11) gives for any $\alpha \in \mathbb{C}$

$$\mathbb{Q}\mathbb{A}\mathbb{P}^{\perp} = -\frac{1}{2}\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}\begin{bmatrix} 1 & -1 \\ \alpha & 0 \end{bmatrix}\begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} = 0 \tag{4.13}$$

From (D) follows that m-sectorial operators are precisely those admitting representation in terms of sesquilinear forms. For a given $\Delta$ parametrized by $\mathbb{Q}, \mathbb{P}, \mathbb{L}$, the corresponding form can be shown [71] to be

$$h[\psi] = \|\psi'\|^2_{\mathcal{G}} + \sum_n \langle \mathbb{L}\mathbb{Q}\psi_n(v)|\mathbb{Q}\psi_n(v)\rangle \qquad \mathfrak{D}(h) = \{\, \psi \in W^{2,2}(\mathcal{G}) \mid \mathbb{P}\psi_n(v) = 0 \,\} \tag{4.14}$$

**Regular boundary conditions**

As long as we are interested in crypto-self-adjoint operators, we do not need to further generalize the m-sectorial conditions, because any crypto-self-adjoint operator bounded below is apparently m-sectorial. Just for the sake of completeness, we consider conditions which are not m-sectorial, but still admit the parametrization in terms of $\mathbb{U}$ and $k$. Such conditions are commonly denoted as *regular*. All m-sectorial conditions are regular, which follows from the fact that the matrix $(\mathbb{L}+\mathbb{P}+ik\mathbb{P}^\perp)$ is invertible for $k > \|\mathbb{L}\|$, and the transformation

$$\mathbb{U}(k) = \left(\mathbb{L}+\mathbb{P}+ik\mathbb{P}^\perp\right)^{-1}\left(\mathbb{L}+\mathbb{P}+ik\mathbb{P}^\perp\right) \tag{4.15}$$

On the other hand, not all regular conditions are m-sectorial: as and example, consider [27]

$$\mathbb{A} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \qquad \mathbb{B} = \begin{bmatrix} 0 & 0 \\ -1 & 0 \end{bmatrix} \tag{4.16}$$

for which the criterion of m-sectoriality (4.11) gives

$$\mathbb{Q}\mathbb{A}\mathbb{P}^\perp = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix}\begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \neq 0 \tag{4.17}$$

while $(\mathbb{A} - ik\mathbb{B})$ is invertible for any $k \in \mathbb{C}$. To make the characterization of boundary conditions complete, we call conditions not satisfying the regularity assumption as *irregular*. Most often, they correspond to pathologically behaved $\Delta$, and example being

$$\mathbb{A} = \begin{bmatrix} 1 & 1 \\ 0 & 0 \end{bmatrix} \qquad \mathbb{B} = \begin{bmatrix} 0 & 0 \\ 1 & 1 \end{bmatrix} \tag{4.18}$$

**Crypto-self-adjoint boundary conditions**

A central task of this section would be obviously to parametrize crypto-self-adjoint boundary conditions. In case that the self-adjoint partner of $\Delta$ is another Laplacian, the problem can be, at least in the case of equilateral graphs, again parametrized by boundary condition matrices. Indeed, it was proven in [27], that whenever there exists a positive $\mathbb{W}$, such that

$$\mathbb{A}\mathbb{W}\mathbb{B}^\dagger = \mathbb{B}\mathbb{W}\mathbb{A}^\dagger \qquad \mathbb{W}\mathbb{U}^{-1} = \mathbb{U}^\dagger\mathbb{W} \qquad \mathbb{W}\mathbb{L} = \mathbb{L}^\dagger\mathbb{W} \tag{4.19}$$

then we can declare $\Delta$ to be crypto-self-adjoint. An example of such boundary conditions would be generalized Robin conditions with $\alpha, \beta, \gamma \in \mathbb{R}$

$$\mathbb{A} = \begin{bmatrix} \alpha & \gamma \\ 0 & \beta \end{bmatrix} \qquad \mathbb{B} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \tag{4.20}$$

In general, however, $\Delta$ may be similar to any conceivable self-adjoint operator. As an example, consider the conditions

$$\mathbb{A} = \begin{bmatrix} i\alpha & 0 \\ 0 & -i\alpha \end{bmatrix} \qquad \mathbb{B} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \tag{4.21}$$

corresponding to the model (3.28). Although there is no positive matrix $\mathbb{W}$ satisfying (4.19), this operator was already shown crypto-self-adjoint, with its self-adjoint counterpart given by (**??**).

## 4.2 Models

The final section of this work introduces several simple models, which provide a framework to apply our crypto-self-adjoint formalism in the case of quantum graphs. Properties of these models shall be illustrated on a star graph with the boundary conditions

$$\begin{aligned} \mathfrak{D}(\Delta_1) &= \left\{ \psi \in W^{2,2}(\mathcal{G}) \;\middle|\; \psi_\varepsilon(0) = 0 \qquad \psi_\varepsilon(d_\varepsilon) = \psi_{\varepsilon'}(d_\varepsilon) \qquad \sum_\varepsilon \psi'_\varepsilon(d_\varepsilon) = \alpha\psi(d_\varepsilon) \right\} \\ \mathfrak{D}(\Delta_2) &= \left\{ \psi \in W^{2,2}(\mathcal{G}) \;\middle|\; \psi'_\varepsilon(0) = 0 \qquad \psi'_\varepsilon(d_\varepsilon) = \psi'_{\varepsilon'}(d_\varepsilon) \qquad \sum_\varepsilon \psi_\varepsilon(d_\varepsilon) = \alpha\psi'(d_\varepsilon) \right\} \end{aligned} \tag{4.22}$$

which are commonly denoted as $\delta$ and $\delta'$ interaction conditions [17]. The matrices (4.4) have a simple form, sampled here for dimension 4 as

$$\mathbb{A}/\mathbb{B} = \begin{bmatrix} 1 & -1 & 0 & 0 \\ 0 & 1 & -1 & 0 \\ 0 & 0 & 1 & -1 \\ 0 & 0 & 0 & -\alpha \end{bmatrix} \qquad \mathbb{B}/\mathbb{A} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 1 & 1 & 1 & 1 \end{bmatrix} \tag{4.23}$$

It can be directly verified using criteria (4.8) and (4.11), that the operators (4.22) are self-adjoint for $\alpha \in \mathbb{R}$ and m-sectorial for any $\alpha \in \mathbb{C}$. The secular equations can be written explicitly as

$$\sum_{\varepsilon} \cot(\kappa d_{\varepsilon}) = \frac{\alpha}{\kappa} \qquad \sum_{\varepsilon} \tan(\kappa d_{\varepsilon}) = -\frac{\alpha}{\kappa} \tag{4.24}$$

### 4.2.1 I: Weighted/gauged Laplacian

Here we present two generalizations of $\Delta$ with abitrary boundary conditions of (4.4) which acquire a natural interpretation in the crypto-self-adjoint formalism. The first one is made by introducing a multiplicative weight function $w_{\varepsilon}$ obeying the inequalities $c > w_{\varepsilon}(x_{\varepsilon}) > c^{-1} > 0$, transforming $\Delta$ into

$$\Delta = -w_{\varepsilon}(x_{\varepsilon}) \frac{d^2}{dx_{\varepsilon}^2} \qquad \mathfrak{D}(\Delta_{min}) \subseteq \mathfrak{D}(\Delta) \subseteq W^{2,2}(\mathcal{G}) \tag{4.25}$$

Such weight function may easily spoil the self-adjointness of $\Delta$, as seen from integrating by parts, e.g. in the model (4.22). It is however a simple observation, that (4.25) can be returned to the self-adjoint framework by introducing a representation space $\mathcal{H}^{(S)}$ with the inner product

$$\langle \phi | \psi \rangle_{\mathbb{W}} = \sum_{\varepsilon} \int_{\varepsilon} \phi^*(x_{\varepsilon}) \psi(x_{\varepsilon}) w^{-1}(x_{\varepsilon}) dx_{\varepsilon} \tag{4.26}$$

Following the recipe of (4.4), we may again truncate such metric operator into matrix form, which provides a definite answer to a question of Laplacian self-adjointness. The truncated metric operator is a diagonal matrix of dimension $\sum d_v$

$$\mathbb{W} = \text{diag}\left[\frac{1}{w_{\varepsilon}(0)}, \frac{1}{w_{\varepsilon}(d_{\varepsilon})}\right] \tag{4.27}$$

As long as $\mathcal{G}$ is a compact graph and the condition $w_{\varepsilon}(x_{\varepsilon}) > c > 0$ holds, such metric is apparently bounded together with its inverse. The case of the weight function may be thus transformed away just as well as crypto-self-adjoint conditions $\Delta$ in (4.19). Moreover, this result can be applied to graphs with inequal edge lengths. If we assume to be constant edgewise $w_{\varepsilon}(x_{\varepsilon})$, we may generalize the secular equation (4.24) into the form

$$\sum_{\varepsilon} \frac{1}{\sqrt{w_{\varepsilon}}} \cot\left(\frac{\kappa d_{\varepsilon}}{\sqrt{w_{\varepsilon}}}\right) = \frac{\alpha}{\kappa} \qquad \sum_{\varepsilon} \frac{1}{\sqrt{w_{\varepsilon}}} \tan\left(\frac{\kappa d_{\varepsilon}}{\sqrt{w_{\varepsilon}}}\right) = -\frac{\alpha}{\kappa} \tag{4.28}$$

Exactly the same recipe may be applied to generalize (4.29) to a compact graph $\mathcal{G}$, with boundary conditions again parametrized as in (4.4)

$$\mathbf{H} = -\mu \frac{d^2}{dx_{\varepsilon}^2} + \frac{d}{dx_{\varepsilon}} \qquad \mathfrak{D}(\Delta_{min}) \subseteq \mathfrak{D}(\Delta) \subseteq W^{2,2}(\mathcal{G}) \tag{4.29}$$

Because the mapping (3.24) remains bounded and boundedly invertible when acting on a compact graph, all the fact shown in (4.29), including the reality and discreteness of spectrum and completeness of eigenfunctions, remain valid. The truncated metric operator (3.24) truncated to the vertices has the form

$$\mathbb{W} = \text{diag}\left[1, \exp\left(\frac{d_{\varepsilon}}{\mu}\right)\right] \tag{4.30}$$

which may be of course freely combined with any weight function of (4.25), resulting again in a diagonal metric. The secular equations (4.24) for the convection-diffusion case read

$$\frac{q}{2\mu} + \frac{1}{2\mu} \sum_{\varepsilon} \cot\left(\frac{\sqrt{1-4\lambda\mu}}{2\mu} d_{\varepsilon}\right) = \frac{\alpha}{\kappa} \qquad \frac{q}{2\mu} + \frac{1}{2\mu} \sum_{\varepsilon} \tan\left(\frac{\sqrt{1-4\lambda\mu}}{2\mu} d_{\varepsilon}\right) = -\frac{\alpha}{\kappa} \tag{4.31}$$

### 4.2.2 II: Complex Robin boundary conditions

This model, introduced in [28], may be seen as a direct generalization of (3.28) from real interval to a compact graph $\mathcal{G}$. For reasons of simplicity, we restrict attention to an equilateral star graph. Denoting the edge length as $L$, number of edges as $q$, and $\phi = 2\pi/q$, we write

$$\mathfrak{D}(\Delta) = \left\{ \psi \in W^{2,2}(\mathcal{G}) \;\middle|\; \psi_\varepsilon(L) = \psi_{\varepsilon'}(L), \quad \sum_\varepsilon \psi'_\varepsilon(L) = 0, \quad \psi'_\varepsilon(0) = \mathrm{i}\alpha \exp(\mathrm{i}\varepsilon\phi)\, \psi_\varepsilon(0) \right\} \tag{4.32}$$

which can be expressed with the help of parametrization (4.4) as

$$\mathbb{A} = \begin{bmatrix} \mathbb{A}' & 0 \\ 0 & \mathbb{A}_\nu \end{bmatrix} \qquad \mathbb{B} = \begin{bmatrix} \mathbb{I} & 0 \\ 0 & \mathbb{B}_\nu \end{bmatrix} \tag{4.33}$$

with $\mathbb{A}_\nu, \mathbb{B}_\nu$ being usual Kirchhoff conditions at the central vertex, expressible as (4.22) with $\alpha = 0$, and

$$\mathbb{A}' = \operatorname{diag}\left[\mathrm{i}\alpha \exp(\mathrm{i}\varepsilon\phi)\right] \tag{4.34}$$

Since, just as in (4.21), the matrix Dieudonné equation does not have any positive solutions, we may conclude that (4.32) is not similar to any self-adjoint Laplacian. The possible similarity to other self-adjoint operators must be examined manually. The secular equation of (4.32) reads

$$\sum_{\varepsilon=0}^{q-1} \frac{\mathrm{i}\alpha \exp(\mathrm{i}\varepsilon\phi) - k\tan(kL)}{\mathrm{i}\alpha \exp(\mathrm{i}\varepsilon\phi)\tan(kL) + k} = 0 \tag{4.35}$$

The sum on the left side admits explicit summation, resulting in a remarkably simple formula

$$q\frac{\kappa^q + (-i\alpha)^q \tan^{q-2}(\kappa L)}{\kappa^q - (i\alpha)^q \tan^q(\kappa L)} \tan(\kappa L) = 0 \tag{4.36}$$

Its roots split into a trivial ($q$-independent) part, given by roots of $\tan(\kappa L) = 0$ and $\cot(\kappa L) = 0$, and non-trivial part given by roots of

$$\kappa^q + (-\mathrm{i}\alpha)^q \tan^{q-2}(\kappa L) = 0 \tag{4.37}$$

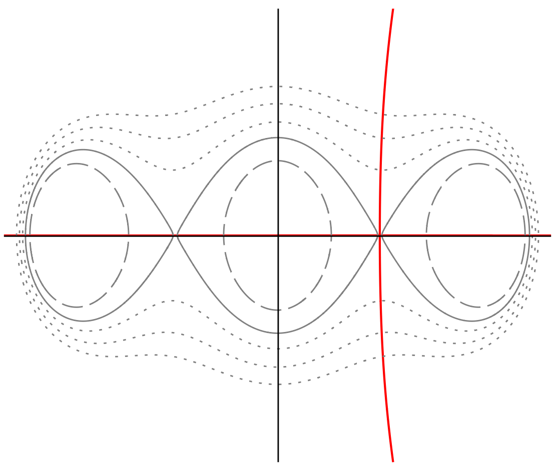

Figure XV: Plots of (4.39) for various $\alpha$ (lower $\alpha$ - dash, higher $\alpha$ - dot)

Solutions of this equation are no longer accessible in explicit form. We shall discuss separately various values of $q$

$$\begin{aligned}
&\bullet \quad q = 4n && \kappa = -\alpha \tan^{\frac{2n-1}{2n}}(\kappa L) \\
&\bullet \quad q = 2n+1 && \kappa = \pm\mathrm{i}\alpha \tan^{\frac{2n-1}{2n+1}}(\kappa L) \\
&\bullet \quad q = 4n+2 && \kappa = \quad \alpha \tan^{\frac{2n}{2n+1}}(\kappa L)
\end{aligned} \tag{4.38}$$

For $q = 4n$ and $q = 2n + 1$, $\mathbf{H}$ can be shown numerically [72] to possess complex eigenvalues for any $\alpha$, which prevents them from being crypto-self-adjoint. For $q = 4n + 2$, by denoting $k = a + ib$ and switching into polar coordinates, we arrive to

$$\frac{2n}{2n+1} \arctan\left(\frac{\sinh(b)\cosh(b)}{\sin(a)\cos(a)}\right) = \arctan\left(\frac{b}{a}\right) \qquad \alpha\left(\frac{\cosh^2(b) - \cos^2(a)}{\sinh^2(b) + \cos^2(a)}\right)^{\frac{2n}{2n+1}} = a^2 + b^2 \tag{4.39}$$

with one of the equations being independent on $\alpha$. We have plotted such implicit equation for various values of $\alpha$ in fig. XV, with the argument equation in red, and the modulus equation in gray. We see that both equations are satisfied for a non-trivial argument only, when $\alpha$ exceeds certain value $\alpha_{crit} \sim 0.7863$. We are even able to determine the location of the point $x_\alpha$. To do this, it suffices to examine singular points (where $\partial_a = \partial_b = 0$) of the leftmost equation in (4.39), which localizes $x_\alpha$ as an unique positive root of the equation

$$\frac{\sin 2a}{2a} = \frac{2n}{2n+1} \tag{4.40}$$

# Conclusion

The constantly growing family of known crypto-self-adjoint operators motivates the study of their physical representation spaces, which is equivalent to the study of their metric operators. Among many approaches for constructing such metric operators, we have established techniques of solving explicitly the Dieudonné equation (1.10), summing the spectral resolution formula (B.8), or transformation into phase space (3.11).

The studied models broadly fall into two families. The first family consists of finite-dimensional $n \times n$ families (2.9), (2.14) and (2.19) studied from the viewpoint of quantum catastrophes. The emergence of characteristic cusp-like shapes of . . . may be seen as a very pleasant phenomenon, which may, in parallel to classical catastrophe theory, prove relevant e.g. in the field quantum phase transitions [54].

The second family contains differential models on intervals and graphs. Special attention should be paid to the elegant model (3.28), where the exceptional simplicity of the operator itself contrasts with the nontrivial form of the corresponding metric operators (3.34). An advection-diffusion model admitting much simpler metric operators (which is however usually not appreciated in relevant literature) has been presented in (4.29). These two examples are finally complemented by an application of the quantum-mechanical interpretation of Klein-Gordon (3.12) and Proca [43] equations, achieved with the help of crypto-self-adjoint formalism (3.21).

In the final part of our considerations, crypto-self-adjoint operators have been has been considered from the viewpoint of quantum graphs. We provided brief review of the central model of interest, Laplacian with the boundary conditions (4.4), with emphasis on operator crypto-self-adjointness. In this field, there is still a wide area of open problems, an example being the graph analogue of the model (3.28), where the crypto-self-adjointness can be conjectured based on considerations from fig. XV.

# Appendix

## A Rigged Hilbert spaces

This section aims to give precise meaning to the notion of generalized eigenvectors, which correspond to continuous spectrum of linear operators. Such eigenvectors by definition do not belong to the Hilbert space $\mathcal{H}$ under consideration, which motivates building an amended structure *around* such $\mathcal{H}$ in the spirit of distribution theory. Such structure is usually called *rigged Hilbert space*. It is defined as a triplet

$$\Phi \subseteq \mathcal{H} \subseteq \Phi^* \tag{A.1}$$

where $\Phi$ is dense in $\mathcal{H}$ with topology inherited from $\mathcal{H}$, and $\Phi^*$ is the continuous dual of $\Phi$ (the second inclusion has to be understood as isomorphic embedding). The subspace $\Phi$ should be chosen as maximal subspace invariant to the action of all observables. Indeed, it can be proven [**?** ], that if we choose the subspace so that $\mathbf{H}(\Phi) = \Phi$, then there exists an unique operator $\mathbf{H}^\dagger : \Phi^* \to \Phi^*$ satisfying

$$\mathbf{H}^\dagger f(\psi) = f(\mathbf{H}\psi) \quad \forall \psi \in \Phi \quad \forall f \in \Phi^* \tag{A.2}$$

where we shall denote $f(\psi) = \langle f|\psi\rangle$. The restriction of $\mathbf{H}^\dagger$ to $\Phi$ corresponds to usual definition of adjoint operator. and consequently $\langle \mathbf{H}^\dagger f|\psi\rangle = \langle f|\mathbf{H}\psi\rangle$. This enables to rigorously define the notion of *generalized eigenvector* of $\mathbf{H}$. It is such $f \in \Phi^*$, that obeys

$$\langle \mathbf{H}^\dagger f|\psi\rangle = \lambda\langle f|\psi\rangle \qquad \forall \psi \in \Phi \tag{A.3}$$

This notion gives a precise meaning to the statement *"eigenvectors of a self-adjoint operator* $\mathbf{H} \in \mathcal{C}(\mathcal{H})$ *form an orthonormal basis of* $\mathcal{H}$*"*: it means that for every $\phi, \psi \in \Phi$, we have

$$\langle \phi|\psi\rangle = \sum_n \langle \phi|f_n\rangle\langle f_n|\psi\rangle = \sum_n \overline{\langle f_n|\phi\rangle}\langle f_n|\psi\rangle \tag{A.4}$$

which shall be expressed throughout this work as

$$\mathbf{I} = \sum_n |f_n\rangle\langle f_n| \tag{A.5}$$

**Example (Schwartz space)**

Consider the space $L^2(\mathbb{R})$ with canonical operators of position and momentum, defined as

$$\begin{aligned} (\mathbf{x}\psi)(x) &= x\psi(x) & \mathfrak{D}(\mathbf{x}) &= \{\, \psi \in L^2(\mathbb{R}) \mid x\psi \in L^2(\mathbb{R}) \,\} \\ (\mathbf{p}\psi)(x) &= \mathrm{i}\frac{d\psi}{dx}(x) & \mathfrak{D}(\mathbf{p}) &= \{\, \psi \in L^2(\mathbb{R}) \mid \psi \in AC(\mathbb{R}) \;\; \psi' \in L^2(\mathbb{R}) \,\} \end{aligned} \tag{A.6}$$

The subspace maximally invariant to the action of both $\mathbf{x}$ and $\mathbf{p}$ can be expressed as

$$\Phi = \bigcap_{n,m=0}^{\infty} \mathfrak{D}(\mathbf{A}^n\mathbf{B}^m) \tag{A.7}$$

which is simply a space invariant to the action of derivative and polynomial multiplication. This is, by definition, the Schwartz space $\mathcal{S}$ [**?** ] of rapidly decreasing functions, which is dense in $L^2(\mathbb{R})$. Its dual space $\mathcal{S}^*$, the space of tempered distributions, contains the generalized eigenvectors of both momentum $\exp(ikx)$ and position $\delta(k-x)$. For any two vectors from $\mathcal{H}$, we have

$$\langle \phi|\psi\rangle = \int_{\mathbb{R}} \langle \phi|k\rangle \overline{\langle \psi|k\rangle} dx = \int_{\mathbb{R}} \mathcal{F}(k)\overline{\mathcal{F}(k)} dk \tag{A.8}$$

which is just the Parseval relation. By means of Fourier transform, the same holds for $\delta(x-k)$.

# B Spectral properties of crypto-self-adjoint operators

It is a well-known fact, that eigenvectors of every self-adjoint operator form an orthonormal basis $(\psi_n)$, in the sense of (A). The notion of orthonormal basis can be (in Hilbert spaces) equivalently expressed as

$$\sum_n |\psi_n\rangle\langle\psi_n| = \mathbf{I} \tag{B.1}$$

For a crypto-self-adjoint operator $\mathbf{H}$, we show that its eigenvectors, despite not being orthogonal, are well-behaved in the sense that they form a *Riesz basis*

$$C^{-1}\mathbf{I} \le \sum_n |\psi_n\rangle\langle\psi_n| \le C\mathbf{I} \tag{B.2}$$

**Proposition** ([27]). $\mathbf{H} \in \mathcal{C}(\mathcal{H})$ *is crypto-self-adjoint, if and only if it has real spectrum and a Riesz basis of eigenvectors.*

*Proof.* The eigenvectors of $\mathbf{h} = \mathbf{\Omega H \Omega}^{-1} = \mathbf{h}^\dagger$ have the form $(\mathbf{\Omega}\psi_n)$ and form an orthonormal basis of $\mathcal{H}$, which means that the Riesz basis property (B.2) of $(\psi_n)$ holds with $C = \max\{\,\|\mathbf{\Omega}\|, \|\mathbf{\Omega}^{-1}\|\,\}$. Conversely, for a given Riesz basis of $\mathcal{H}$, which we denote $(\psi_n)$, construct an operator

$$\mathbf{L} = \sum_n \alpha_n |\psi_n\rangle\langle\psi_n| \tag{B.3}$$

with $\alpha_n$ being arbitrary positive constants. This operator is manifestly positive, and the Riesz property implies that it is also bounded and boundedly invertible. Furthermore, the identity

$$\sum_n \alpha_n |\psi_n\rangle\langle\psi_n|\mathbf{H}^\dagger = \sum_n \alpha_n\lambda_n^* |\psi_n\rangle\langle\psi_n| = \sum_n \alpha_n\lambda_n |\psi_n\rangle\langle\psi_n| = \mathbf{H}\sum_n \alpha_n |\psi_n\rangle\langle\psi_n| \tag{B.4}$$

shows that the Dieudonné equation holds holds with $\mathbf{\Theta} = \mathbf{L}^{-1}$. □

In order to generalize the usual spectral resolution formulas for crypto-self-adjoint operators, we introduce the notion of *biorthonormal basis*, a system $(\psi_n, \phi_n)$ satisfying $\langle \psi_m|\psi_n\rangle = \delta_{mn}$. In a Hilbert space, this again admits and equivalent expression

$$\sum_n |\psi_n\rangle\langle\phi_n| = \mathbf{I} \tag{B.5}$$

It can be proven [? ], that for a given family $(\psi_n)$, the biorthogonal basis $(\psi_n, \phi_n)$ exists if and only if $(\psi_n)$ is a Riesz basis. and from the formula

$$\lambda_n\langle\psi_n|\phi_m\rangle = \langle \mathbf{H}\psi_n|\phi_m\rangle = \langle\psi_n|\mathbf{H}^\dagger\phi_m\rangle = \lambda_m\langle\psi_n|\phi_m\rangle \tag{B.6}$$

that such system could be chosen as biorthogonal complement for $\psi_n$ is formed precisely of eigenvectors of $\mathbf{H}^\dagger$. The spectral resolution of the former operator and its adjoint can be written as

$$\mathbf{H} = \sum_n \lambda_n |\psi_n\rangle\langle\phi_n| \qquad \mathbf{H}^\dagger = \sum_n \lambda_n |\phi_n\rangle\langle\psi_n| \tag{B.7}$$

The formula for $\mathbf{\Theta}^{-1}$ has already been shown in (B.3) it is a genuine question to ask for spectral resolutions for the operators $\mathbf{\Theta}$ and $\mathbf{\Omega}$.

$$\mathbf{\Theta} = \sum_n \alpha_n |\phi_n\rangle\langle\phi_n| \qquad \mathbf{\Theta}^{-1} = \sum_n \alpha_n |\psi_n\rangle\langle\psi_n| \qquad \alpha_n > 0 \tag{B.8}$$

# C Crypto-self-adjointness and antilinear symmetries

A concept closely related to crypto-self-adjointness is that of having an antilinear symmetry. We say that $\mathbf{H} \in \mathcal{C}(\mathcal{H})$ possesses an *antilinear symmetry*, if an antilinear bijection $\mathbf{A}$ exists, such that $[\mathbf{H}, \mathbf{A}] = 0$. Every crypto-self-adjoint operator can be shown to possess an antilinear symmetry [73]. Although antilinear symmetry does not quarantee reality of the spectrum by itself, it is sufficient to establish conjugate invariance of the spectrum, which follows from the definition of spectrum and

$$(\mathbf{H} - \lambda^*)^{-1} = \mathbf{A}^{-1}(\mathbf{H} - \lambda)^{-1}\mathbf{A} \tag{C.1}$$

and the fact that everywhere defined operators $\mathbf{A}$ and $\mathbf{A}^{-1}$ are necessarily bounded. A special case of an antilinear symmetry is $\mathcal{PT}$-symmetry, in which the antilinear operator $\mathcal{PT}$ admits a decomposition into a linear operator of parity $\mathcal{P}$ and antilinear operator of time-reversal $\mathcal{T}$, such that

$$\mathcal{P}^2 = \mathcal{T}^2 = \mathbf{I} \qquad [\mathcal{P}, \mathcal{T}] = 0 \tag{C.2}$$

Such operators are tranditionally chosen on $L^2(\mathbb{R})$ to be

$$(\mathcal{P}\psi)(x) = \psi(-x) \qquad (\mathcal{T}\psi)(x) = \psi(x)^* \tag{C.3}$$

thus justifying their names. It can be shown [73] that any $\mathcal{PT}$-symmetric operator is self-adjoint in a *Krein space*, that is a vector space $\mathcal{V}$ equipped with a sesquilinear form $h(.,.)$, which admits a decomposition $\mathcal{V} = \mathcal{V}_+ \bigoplus \mathcal{V}_-$, such that

$$h(\psi_+, \psi_-) = 0 \qquad \psi_\pm \in \mathcal{V}_\pm \tag{C.4}$$

Any Krein space $\mathcal{V}$ can be promoted to a Hilbert space by introducing an inner product in terms of projections onto $\mathcal{V}_\pm$ and an involutive operator $\mathcal{J} = \mathcal{P}_+ - \mathcal{P}_-$ as

$$\langle\psi|\phi\rangle = h(\phi|\mathcal{J}\psi) = h(\psi|\mathcal{P}_+\phi) - h(\psi|\mathcal{P}_-\phi) \geq 0 \tag{C.5}$$

The metric operator for such $\mathbf{H}$ is usually sought for with the help of the so-called *charge operator* $\mathcal{C}$, which is nothing more than the fundamental Krein space symmetry $\mathcal{J}$. The metric operator in this case is found to be $\mathcal{CP}$ [16].

# D Sectorial forms and operators

It is well known [3] that there is a 1-to-1 correspondence between bounded operators $\mathbf{H} \in \mathcal{B}(\mathcal{H})$ and bounded, everywhere defined sesquilinear forms on $\mathcal{H}$. This correspondence can be broadened to a correspondence between sectorial forms and m-sectorial operators, by means of famous Kato's representation theorem [4]. M-sectorial operator may be seen as a generalization of self-adjoint Hamiltonians, which still obey the fundamental physical requirement of boundedness from below. To state the representation theorem, we need several auxiliary notions. A *numerical range* of a closed operator $\mathbf{H} \in \mathcal{C}(\mathcal{H})$ is a subset of complex plane, defined as

$$\Theta(\mathbf{H}) = \{\, \langle\psi|\mathbf{H}|\psi\rangle \mid \|\psi\| = 1 \,\} \tag{D.1}$$

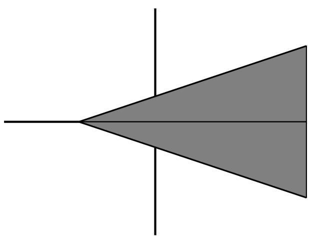

Figure XVI: Numerical range of a sectorial operator

A linear operator $\mathbf{H} \in \mathcal{C}(\mathcal{H})$ or a sesquilinear form $h(\phi, \psi)$ on $\mathcal{H}$ are called *sectorial*, if their numerical range lies in some sector around a positive real axis, i.e. there exist such constants $\mu, \theta \in \mathbb{R}$ such that

$$\Theta(\mathbf{H}) \subset \left\{\lambda \in \mathbb{C} \mid \operatorname{Re}\lambda \geq \mu, \ \ |\arg(\lambda - \mu)| \leq \theta\right\} \tag{D.2}$$

For the definition of a *m-sectorial operator*, we moreover impose a condition of certain well-behavedness on the resolvent. This condition is usually *quasi-m-accretivity* in elliptic operator theory.

$$\|(\mathbf{H} + \alpha - \lambda)^{-1}\| \leq \frac{1}{|\operatorname{Re}\lambda|} \tag{D.3}$$

An operator obeying both (D.3) and (D.2) is called *m-sectorial*. It is precisely this family of operators that admits equivalent representation in terms of quadratic forms.

**Theorem** ([4]). *Let $h(\phi, \psi)$ be a closed and sectorial sesquilinear form in $\mathcal{H}$. Then there exists a corresponding unique m-sectorial operator, such that*

$$\begin{aligned} &\bullet \quad \mathfrak{D}(\mathbf{H}) \subset \mathfrak{D}(h) \\ &\bullet \quad \phi \in \mathfrak{D}(h), \psi \in \mathcal{H} \implies \phi \in \mathfrak{D}(\mathbf{H}), \mathbf{H}\phi = \psi \end{aligned} \tag{D.4}$$

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