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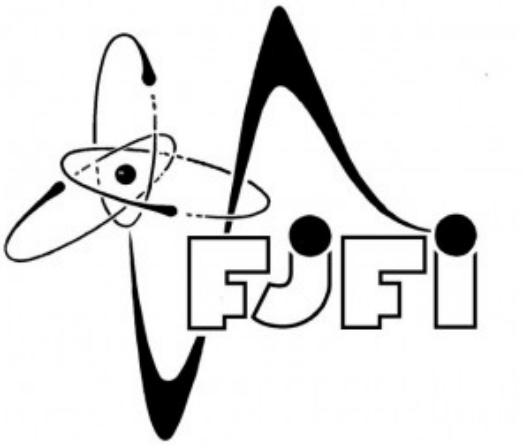

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Non-Selfadjoint Operators in Quantum Physics: Selected Aspects

Supervisor: Miloslav Znojil DrSc.
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I declare that I carried out this thesis independently and only with the cited literature and other professional sources.

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Název práce: **Nesamosdružené operátory v kvantové fyzice: vybrané aspekty**

Autor: František Růžička

Katedra: Katedra fyziky

Vedoucí práce: Miloslav Znojil DrSc.

Abstrakt: Práce se zabývá reprezentací kvantových pozorovatelných pomocí nesamosdružených operátorů, pro niž se v literatuře vžil název kvazi-hermitovská kvantová mechanika. Těžiště této teorie spočívá v konstrukci dynamické metriky (a tím i fyzikálního Hilbertova prostoru) pro daný Hamiltonián či jinou pozorovatelnou. V této práci je analyticky vyšetřováno několik typů konečně-dimenzionálních a diferenciálních Hamiltoniánů, pro něž je možné přesně vyřešit problém konstrukce univerzální metriky.

Klíčová slova: nesamosdruženost, metrika, reprezentace kvantové mechaniky, diskrétní kvantová mechanika, Su-Schrieffer-Heeger, pseudospektrum

Title: **Non-selfadjoint operators in quantum physics: selected aspects**

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Abstract: The present thesis deals with a representation of quantum observables using non-hermitian operators, which is usually referred to as quasi-hermitian quantum mechanics. The core of this representation lies in the construction of a dynamical metric (and consequently of a physical Hilbert space) for a given non-hermitian observable. This thesis deals with analytical examination for several families of both finite-dimensional and differential Hamiltonians, which admit an exact construction of the universal metric.

Keywords: non-hermitian operators, metric, representations of quantum mechanics, discrete quantum mechanics, Su-Schrieffer-Heeger, pseudospectrum

Contents

Prologue

Since the early days of quantum mechanics, observables are traditionally associated with hermitian operators. This has obviously very good and deep-rooted reasons, the reality of the spectrum and the unitarity of time evolution. For a very long time, it seemed impossible and absurd that an observable quantity could be ever represented by a non-hermitian operator. Of course, the appearance of such operators in quantum mechanics per se is not new at all: they are routinely used e.g. to describe resonances [1] or open dissipative systems [2].

The paradigm began to change slowly in the early 90s, in particular with the work of the Stellenbosch group, nicely summarized in an influential paper [3]. After several years of stagnation, the field obtained a vital impulse in 1998 through the work of Bender and Boettcher [4], with their unexpected claim about the imaginary cubic oscillator. Since this moment, non-hermitian observables presumably entered the world of mainstream physics. The theory was quickly termed "$\mathcal{PT}$-symmetric quantum mechanics", because of the initial consensus that $\mathcal{PT}$-symmetry was the governing principle behind the reality of the spectrum. After some years, however, it became clear that such claim was an oversimplification, and the general mechanism is more subtle. Although the term $\mathcal{PT}$-symmetry remains widely used even today, most authors decided instead to call the newly emerged theory "quasi-hermitian quantum mechanics" [5, 6].

Applications of quasi-hermitian theory form also an integral part of the current thesis. In order to make it self-contained, the thesis also compactly reviews the fundamentals of the theory and its current state of art. Since the field is nowadays spanning a wide area of both physics and mathematics, it is alas not possible to cover it as a whole in a single work (hence "selected aspects" in the title). The aspects chosen for review are discussed in the first two chapters. The first chapter reviews the foundations of the theory in more detail that it is usually done, while the second chapter deals with the concept of solvability and its discrete as well as differential realizations. An interested reader looking for a more wide-ranging review manuscript should consult a great recent collection [7].

The final two chapters, on the other hand, are devoted to various results of the present author from the period of last two years. These can be found in five published works so far. While [8, 9, 10] stem from a fruitful collaboration with M. Znojil, the papers [11, 12] are a result of the author's own research in finite-dimensional quasi-hermitian theory. Much of the work presented here owns a lot to the latest generation of mathematical computer software. For all routines involving manipulation with matrices (which is a central problem in the third chapter), MAPLE's symbolic manipulation packages have proven especially fruitful. For plots of operator pseudospectra, a fast and stable plugin for the Matlab suite is available online under the name EigTool [13].

Chapter 1

Non-hermitian operators as quantum observables

1.1 Non-relativistic quantum mechanics

Quasi-hermitian theory was, in its original formulation, first applied to non-relativistic quantum mechanics (although its applications are currently far more wide-ranging). Being commonly tied together with the Hilbert space formulation, we have decided to include also comparison with the phase space and path integral formulations, which have been so far seldom discussed in dedicated literature.

1.1.1 Hilbert space formulation

When considering observables in quantum theories, the usual requirement of hermicity is supported by two well-founded (and closely related) arguments. First, the mean values corresponding to actual measurement outcomes are required to be real quantities (equivalently, the observables under consideration need to have real spectrum). Second, the time evolution of the system is required to be unitary, a condition corresponding to the local conservation of probability. The unitarity of time evolution is strictly equivalent to the hermicity of its generator (the Hamiltonian), which is clearly established by Stone's theorem ([14], thm. 5.9.2)

However, we can object that there exist many non-hermitian operators with real spectrum, which can in principle correspond to quantum measurements. The role of such operators is precisely the source of possible misunderstandings, which quasi-hermitian theory aims to exploit. And indeed, as demonstrated by the success of the theory, using non-hermitian operators with real spectra can lead to intriguing results.

Operators aiming to describe quantum observables must definitely obey one additional condition, the requirement of diagonalizability. Without this condition, the operator necessarily lacks a certain number of eigenvectors, which would lead into problems in its probabilistic interpretation (as the system cannot degenerate to such eigenstate by any measurement process). A simpler and (under certain assumptions) equivalent condition to diagonalizability is hermitizability, the existence of an operator Ω satisfying

$$h = \Omega H \Omega^{-1} = (\Omega H \Omega^{-1})^\dagger = h^\dagger \tag{1.1}$$

While this condition is simple in theory, its verification could be often laborious or even impossible, as the operator Ω is in most cases intractable by constructive methods. An equivalent and even simpler condition can be constructed by manipulating the expression above. By denoting $\Theta = \Omega^\dagger \Omega$, we might express eq. 1.1 as

$$H^\dagger \Theta = \Theta H \tag{1.2}$$

As long as we find a positive Θ satisfying eq. 1.2 for a given non-hermitian H, we can safely promote such operator to a representation of quantum observable. Operators satisfying this condition are usually called quasi-hermitian (although other conventions exist, see e.g. [15]). From the conceptual viewpoint, Θ actually redefines the very notion of the Hilbert space inner product (ϕ, ψ) as

$$(\phi, \psi)_\Theta = (\phi, \Theta\psi) \tag{1.3}$$

in a way making the considered Hamiltonian hermitian. From the strictly mathematical point of view, the operator Θ is required to be bounded and non-singular in order to avoid possible pathologies. However, this condition is often relaxed in the literature, as many physically relevant models satisfy eq. 1.2 with Θ unbounded or singular [4, 16]. Attempts to develop rigorous mathematical formalism for such generalized quasi-hermitian operators also exist, and are actively discussed [17, 18, 19].

To summarize our considerations, any given quasi-hermitian operator may be always rendered hermitian either by modifying the inner product through Θ, or the Hilbert space structure (the wavefunctions) through Ω. In the language of [20], we might describe quasi-hermitian theory by a triplet of Hilbert spaces, shown in fig. I.

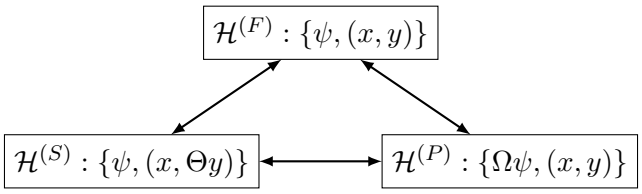

Figure I: *Three Hilbert spaces of quasi-hermitian theory. The space $\mathcal{H}^{(F)}$ is easy to describe but unphysical, while the physical spaces $\mathcal{H}^{(S)}$ and $\mathcal{H}^{(T)}$ can be obtained by modifying eighter the wavefunctions or the inner product.*

The spaces $\mathcal{H}^{(S)}$ and $\mathcal{H}^{(T)}$ are the two (physical) Hilbert spaces obtained by modifying the wavefunctions by Ω, or the inner product by Θ. However, the actual space used to describe a quasi-hermitian operator is the (unphysical) space $\mathcal{H}^{(F)}$, which makes the operator appear non-hermitian. The motives for describing a given operator in $\mathcal{H}^{(F)}$ might be guided by mathematical and computational simplicity, and such operators may also arise naturally in applications.

1.1.2 Phase space formulation

Quantum mechanics formulated in the phase space [21] emerged first (independently) in the works of Weyl [22] and Wigner [23] in the 1930s. Their work was completed some fifteen years later again independently by Groenewold [24] and Moyal [25], who have realized that the Weyl and Wigner mappings are actually inverse to each other, and who introduced the crucial notion of the star product.

We use the lowercase letters $f(x,p)$ to denote phase-space functions and uppercase letters F for Hilbert-space operators. The mappings of Weyl and Wigner between a $2n$-dimensional phase space, and a (unique up to isomorphism) infinite-dimensional Hilbert space bearing a unitary representation of the Heisenberg algebra are

$$\begin{aligned} \text{Weyl:} \qquad f(x,p) &= \frac{1}{2\pi\hbar}\int_{\mathbb{R}^n} dy\, e^{-2ip\cdot y/\hbar}\langle x+y|F|x-y\rangle \\ \text{Wigner:} \qquad \langle x|F|y\rangle &= \frac{1}{2\pi\hbar}\int_{\mathbb{R}^n} dp\, e^{ip\cdot(x-y)/\hbar} f\left(\frac{x+y}{2},p\right) \end{aligned} \tag{1.4}$$

The phase-space analogue of the density matrix is played by its Wigner transform, also called Wigner quasi-probability distribution $\rho(x,p,t)$. If we denote the Weyl-Wigner isomorphism as $f(x,p) \leftrightarrow F$, we see already from the definition that $x \leftrightarrow X$ and $p \leftrightarrow P$. Next, we aim to derive a condition of hermicity in the phase space. Since the operators $U(x,t) = e^{itP}e^{isX}$ form a complete set in the Hilbert space, we may expand any operator as

$$H = \int ds\, dt\, a(t,s) e^{itP} e^{isX} \tag{1.5}$$

We expand the adjoint operator $H^\dagger$ in the same fashion and denote its corresponding function as $a^\dagger(t,s)$. Using the canonical commutation relations for the integrand and comparing it to the result of taking the adjoint directly yields

$$\begin{aligned} H^\dagger &= \int ds\, dt\, a^\dagger(t,s) e^{itX} e^{isP} = \\ &= \int ds\, dt\, a^\dagger(t,s) e^{its} e^{itP} e^{isX} = \int ds\, dt\, a^*(t,s) e^{-itP} e^{-isX} \end{aligned} \tag{1.6}$$

showing that $a^\dagger(t,s) = a^*(-t.-s)e^{-its}$. Finally, by expanding (in a completely analogous fashion) the phase space functions instead of operators and requiring that $h = h^\dagger$, we reveal the phase space hermicity condition to be

$$\begin{aligned} h(x,p) = h^\dagger(x,p) &= \int ds\, dt\, a^\dagger(t,s) e^{itp} e^{isx} = \\ &= \int ds\, dt\, a^*(-t,-s) e^{-its} e^{itp} e^{isx} = e^{i\partial_x\partial_p} h^*(x,p) \end{aligned} \tag{1.7}$$

In order to make the quantum interpretation complete, it remains to define a phase space analogue of operator multiplication. It is obvious, that such an operation must be non-commutative, and therefore may not be played by pointwise function multiplication. Additionally,

such operation should respect the Wigner-Weyl isomorphism, which is formalized in the notion of a $\star$-product, any mapping $\star : \mathbb{R}^n \times \mathbb{R}^n \longrightarrow \mathbb{R}^n$ satisfying

$$FG \leftrightarrow f(x,p) \star g(x,p) \tag{1.8}$$

whenever $F \leftrightarrow f(x,p)$ and $G \leftrightarrow g(x,p)$. A concrete (although not unique) realization of the $\star$-product is commonly implemented by the notion of Moyal product (where we make $\hbar$ appear explicitly, since it shall serve as an expansion parameter)

$$\begin{aligned}(f \star g)(x,p) &= f(x,p) \exp\left(\frac{i\hbar}{2}(\overleftarrow{\partial_x}\overrightarrow{\partial_p} - \overleftarrow{\partial_p}\overrightarrow{\partial_x})\right) g(x,p) = \\ &= \sum_{n=0}^{\infty} \frac{1}{n!}\left(\frac{i\hbar}{2}\right)^n \sum_{k=0}^{n} (-1)^k \binom{n}{k} \frac{\partial^n f(x,p)}{\partial x^k \partial p^{n-k}} \frac{\partial^n g(x,p)}{\partial p^k \partial x^{n-k}}\end{aligned} \tag{1.9}$$

It can be readily seen, that $f \star g = fg + O(\hbar)$, and the Moyal product has a correct classical limit $\hbar \to 0$. The analogue of the commutator (the antisymmetrization of the Moyal product) is called Moyal bracket $\{\{f,g\}\} = \frac{1}{i\hbar}(f \star g - g \star f)$. This bracket may be also expanded in the powers of $\hbar$, yielding

$$\{\{f,g\}\} = \sum_{n=0}^{\infty} \sum_{k=0}^{n} \frac{(-i\hbar)^n (-1)^k}{2^n n!} \binom{n}{k} \frac{\partial^n f(x,p)}{\partial x^k \partial p^{n-k}} \frac{\partial^n g(x,p)}{\partial p^k \partial x^{n-k}} = \{f,g\} + O(\hbar^2) \tag{1.10}$$

with $\{f,g\}$ being the classical Poisson bracket. The Moyal bracket, together with the Wigner quasi-probability distribution $\rho(x,p,t)$, may be used to define the time evolution equation, analogous to the von Neumann equation in Hilbert space

$$\frac{\partial \rho(x,p,t)}{\partial t} = -\{\{\rho(x,p,t), h(x,p,t)\}\} \tag{1.11}$$

where $h(x,p,t)$ denotes the phase-space Hamiltonian, which is commonly required to be hermitian in the sense of eq. 1.7. With this equation at hand, we have expressed all postulates of quantum theory in the phase space, making the analogy complete.

Quasi-hermicity in the phase space

Using the phase space formulation may in general prove very effective for manipulation with certain operators, and quasi-hermitian theory is no exception [26]. The primary reason is, that eq. 1.2 becomes a partial differential equation instead of an operator identity (which allows the application of a whole new class of theorems and numerical methods)

$$h^*(x,p,t) \star \theta(x,p) = \theta(x,p) \star h(x,p,t) \tag{1.12}$$

where we are searching for a phase-space positive function $\theta(x,p)$, given the knowledge of a Hamiltonian function $h(x,p,t)$. We illustrate this framework on perturbative construction of a metric for the imaginary cubic oscillator [27]. This model, despite being in the center

of attention for almost twenty years, is still subject to active research (as demonstrated, for example, by the recent no-go theorem establishing the necessarily unbounded or singular nature of its metrics [28]). Its Hilbert-space Hamiltonian

$$(H\psi)(x) = -\psi''(x) + igx^3\psi(x) \tag{1.13}$$

cannot be solved exactly, and perturbative methods have to be used for computing both its spectrum and its metric. A crucial feature of phase space quasi-hermitian theory is, that the resulting master differential equation has a finite order, whenever $h(x,p)$ depends polynomially on x and p. This is precisely our case, since transforming eq. 1.13 into the phase space results into an equation

$$\begin{aligned} 2ig\,\theta(x,p) - 3gx^2\,\theta_p(x,p) - 3igx\,\theta_{pp}(x,p) + \\ + g\,\theta_{ppp}(x,p) - 2ip\,\theta_x(x,p) + \theta_{xx}(x,p) = 0 \end{aligned} \tag{1.14}$$

Solving this equation perturbatively is much easier compared to its operator equivalent. Still, the general solution is quite complicated even to first order of precision. We make use of the results of [27], and choose a particularly physically appealing solution, which is (up to first order in g)

$$\theta(x,p) = 1 + g\left(\frac{3ix}{4p^4} - \frac{3x^2}{4p^3} - \frac{ix^3}{2p^2} + \frac{x^4}{4p}\right) \tag{1.15}$$

The fact, that this expression indeed solves eq. 1.14, is then verified by simple insertion. The phase space positivity of such a function is equivalent to hermicity of its logarithm $\ln\theta^*(x,p) = e^{-i\partial_x\partial_p}\ln\theta(x,p)$. This may be again verified directly, by expanding to the first order with the result

$$\ln\theta(x,p) = g\left(\frac{3ix}{4p^4} - \frac{3x^2}{4p^3} - \frac{ix^3}{2p^2} + \frac{x^4}{4p}\right) \tag{1.16}$$

Indeed, the constructed solution $\theta(x,p)$ is positive and thus a genuine metric. In general, constructing positive of solutions of eq. 1.12 is a highly nontrivial problem, and it is always nice to have even a single such solution at hand. In such case, the remaining solutions can be treated as small perturbations while preserving the positivity condition.

1.1.3 Path integral formulation

The final one in the triumvirate of basic quantum-theoretical frameworks is obviously the path integral formulation. While the Hilbert space and phase space formulations are closely related through the correspondence of Wigner and Weyl, the path integral approaches quantum theory from a fundamentally different perspective, making analogies with the former often subtle and well disguised. Instead of the Hamiltonian, the fundamental object in the path-integral formalism is the n-point correlation function (also called the correlator) defined as

$$G_n(t_1,\dots,t_n) = \langle\Omega|T\left\{x(t_1),\dots,x(t_n)\right\}|\Omega\rangle = \\ = \frac{\int \mathcal{D}x\; x_1\dots x_n\; e^{iS[x]}}{\int \mathcal{D}x\; e^{iS[x]}} \tag{1.17}$$

where the integral has to be understood as an appropriatelly regularized sum over paths from $-\infty$ to $+\infty$ (for a more mathematically appealing definition, we refer to any textbook on the subject [29]). The correlators may be obtained as expansion coefficients of a so-called generating functional

$$Z[J] = \int \mathcal{D}x\; e^{iS[x]+i\int dt\; J(t)x(t)} \tag{1.18}$$

with respect to the auxiliary (Schwinger) source term $J(x)$ around zero. Note that since we are dealing with functionals (functions over infinite-dimensional spaces), the usual partial derivatives have to be replaced by more general functional derivatives, which can be defined on any Banach space. The correlators may be then expressed as

$$G_n(t_1,\dots,t_n) = \frac{(-i\hbar)^n}{Z[0]}\frac{\delta^n Z[J]}{\delta J[x(t_1)]\dots\delta J[x(t_n)]}\bigg|_{J=0} \tag{1.19}$$

The equations of motion for the correlators may be derived easily from the requirement of invariance, which the generating functional has to satisfy with respect to transformations $x \to x+\varepsilon$. Since the measure $\mathcal{D}\phi$ is invariant *per se*, the condition of invariance up to first order in ε may be written as

$$\int \mathcal{D}x\; e^{iS[x]+\int Jx}\left(i\frac{\delta S}{\delta x(t)} + iJ(t)\right) = \left\langle i\frac{\delta S}{\delta x(t)} + iJ(t)\right\rangle_J = 0 \tag{1.20}$$

This general equation of motion is commonly known under the name Schwinger-Dyson equation. It's in fact an infinite set of coupled equations for correlators of increasing order. These equations may be again obtained by Taylor expanding eq. 1.20 with respect to $J(t)$ around zero. For example, the second coefficient is

$$\begin{aligned} 0 &= \frac{\delta}{\delta J(t)}\frac{\int \mathcal{D}x\; e^{iS[x]+i\int Jx}\left(i\frac{\delta S}{\delta x(t_0)} + J(t_0)\right)}{\int \mathcal{D}x\; e^{iS[x]}}\bigg|_{J=0} = \\ &= \frac{\int \mathcal{D}x\; e^{iS[x]}\left(ix(t)\frac{\delta S}{\delta x(t_0)} + \delta(t-t_0)\right)}{\int \mathcal{D}x\; e^{iS[x]}} = \\ &= i\left\langle\Omega\middle|T\left\{x(t)\frac{\delta S}{\delta x(t_0)}\right\}\middle|\Omega\right\rangle + \delta(t-t_0) \end{aligned} \tag{1.21}$$

Recalling that $\delta S/\delta x(t)$ is equivalent to the operator $L = \frac{d}{dt}\frac{\partial}{\partial\dot{x}} - \frac{\partial}{\partial x}$ acting on $x(t)$, this result demonstrates, that the two-point correlator is actually the (causal) Green's function of the

Lagrange operator. Higher coefficients may be computed analogically using higher functional derivatives, resulting in

$$\begin{aligned} 0 = i\left\langle \Omega \middle| T\left\{ \frac{\delta S}{\delta x(t)}\, x(t_1)\dots x(t_n) \right\} \middle| \Omega \right\rangle + \\ + \sum_{j=1}^{n} \langle \Omega | T\left\{ x(t_1)\dots x(t-t_j)\dots x(t_n) \right\} | \Omega \rangle \end{aligned} \tag{1.22}$$

Path integral and quasi-hermicity

When trying to formulate quasi-hermitian theory in the path integral formalism, the main issue lies in elucidating the role of the metric operator, which may be not *a priori* clear from the outset. We follow [30] and [31, 32], and write the generating functional using the Hamiltonian (instead of the Lagrangian) as

$$\begin{aligned} Z[J] = \int \mathcal{D}x\, \exp\left[-i \int (H - Jx)\, dt \right] = \\ = \mathrm{tr}\left[\exp\left\{ -i \int (H - Jx)\, dt \right\} \right] \end{aligned} \tag{1.23}$$

In the first expression in terms of path integral, H and x are functions, whereas in the second (canonical) term, they are Hilbert space operators. We work with the latter expression in order to demonstrate the presence of the metric operator. Consider H to be quasi-hermitian with respect to a certain Θ. The definition of generating functional remains unchanged. However, the hermitian operator x does no longer play the role of position and must be modified to a quasi-hermitian operator X, so that eq. 1.23 becomes

$$Z[J] = \mathrm{tr}\left[\exp\left\{ -i \int (H - JX) dt \right\} \right] \tag{1.24}$$

This is the correct generating functional of the theory, sufficient to deduce all physical quantities. Since X is quasi-hermitian with respect to the same metric Θ as the Hamiltonian, we may use the decomposition $\Theta = \Omega^\dagger \Omega$ and the cyclic property of the trace to express the functional in terms of canonical position $x = \Omega^{-1} X \Omega$ and hermitian isospectral partner of the Hamiltonian $h = \Omega^{-1} H \Omega$ as

$$Z[J] = \mathrm{tr}\left[\exp\left\{ -i \int (h - Jx) dt \right\} \right] \tag{1.25}$$

Any of the two above functionals may be computed also from the path integral, using the classical analogues of the position and Hamiltonian. Alas, the explicit appearance of either Θ or Ω is the functionals indicate, that the picture has not been simplified in any way by using path integral. Indeed, we still bear the burden of having to find the metric operator or a isospectral hermitian Hamiltonian before applying this machinery. However, as long as we are able to compute these quantities, we might readily express the correlators as

$$G_n(t_1,\ldots,t_n) = \frac{(-i\hbar)^n}{Z[0]} \frac{\delta^n Z[J]}{\delta J[x(t_1)]\ldots\delta J[x(t_n)]}\bigg|_{J=0} = \\ = \langle\Omega|\Theta T\left\{x(t_1),\ldots,x(t_n)\right\}|\Omega\rangle \tag{1.26}$$

As for the evolution equations, using the same invariance condition as in the hermitian scenario (and subsequently performing the functional derivatives) leads to the Schwinger-Dyson equations in a completely same form as in eq. 1.22.

1.2 Relativistic quantum mechanics

Relativistic single-particle quantum mechanics is a theory initially thought to provide synthesis between quantum mechanics and special relativity. However, it was soon found to be plagued with problems and controversies, and abandoned in favor of quantum field theory. Nevertheless, the subject remains relevant even today, mainly because of the gradually increasing interest in theories of quantum gravity, where the field theory approach does not work due to renormalization problems.

Relativistic quantum mechanics is also the subject of one of the most fundamental applications of quasi-hermitian theory. Indeed, the framework helped to resolve a decades-old problem of assigning probabilistic interpretation to certain relativistic quantum equations of motion. We shall discuss details of this procedure for the two most frequently encountered cases: the Klein-Gordon and Proca equation.

1.2.1 The Klein-Gordon equation

The Klein-Gordon equation [33, 34] describes time evolution of relativistic scalars (particles with zero spin). Interestingly, it was written down by Schrödinger even before his more famous eponymous equation. However, it was discarded from quantum-mechanical considerations due to a problem with the non-existence of a positive probability density. We shall consider the Klein-Gordon equation in the absence of external potential

$$\left(\Box + m^2\right)\psi(x,t) = 0 \tag{1.27}$$

Being second-order in time, this equation may look substantially different from the non-relativistic Schödinger equation. It is however a classical result [35], that it may be transformed into a Schrödinger-like canonical form on a space $L^2(M)\oplus L^2(M)$ (provided that $\psi(x,t)$ acts on $L^2(M)$). The transformation can acquire different (but unitarily equivalent) forms, see for example [36] and [37]. We use the parametrization of the former paper, for which we denote $D = -\Delta + m^2$. The Klein-Gordon equation may be then expressed as $i\dot{\Psi}(x,t) = H\Psi(x,t)$ with

$$\Psi(x,t) = \begin{bmatrix} i\dot{\psi}(x,t) \\ \psi(x,t) \end{bmatrix} \qquad H = \begin{bmatrix} 0 & D \\ I & 0 \end{bmatrix} \tag{1.28}$$

The only apparent drawback of this transformation is, that the resulting Hamiltonian is manifestly non-hermitian in the preselected space $L^2\oplus L^2$ (which is a general feature, independent

on the chosen parametrization). Since the free Klein-Gordon equation is known to have a real spectrum $\sigma = (-\infty, +\infty)$, a remedy to this problem may be sought using quasi-hermitian theory.

We aim to construct a metric operator for eq. 1.28 in order to establish its quasi-hermicity. There are several ways to do that, the most direct one being to sum explicitly the series $(\Theta\psi)(x) = \sum \alpha_k \phi_k(x)(\phi_k, \psi)$, where $\phi_k(x)$ are the eigenvectors of the operator $H^\dagger$ and $\alpha_k > 0$ are arbitrary. Restricting attention to operators respecting the block structure of eq. 1.28, we are left with

$$\Theta = \alpha_+ \begin{bmatrix} 1 & -D^{1/2} \\ -D^{1/2} & D \end{bmatrix} + \alpha_- \begin{bmatrix} 1 & D^{1/2} \\ D^{1/2} & D \end{bmatrix} = (\alpha_+ + \alpha_-) \begin{bmatrix} 1 & \frac{\alpha_- - \alpha_+}{\alpha_+ + \alpha_-} D^{1/2} \\ \frac{\alpha_- - \alpha_+}{\alpha_+ + \alpha_-} D^{1/2} & D \end{bmatrix} \tag{1.29}$$

with $D^{1/2}$ defined as the positive square root of the (positive) operator D. Finally, we can denote $\alpha = \frac{\alpha_- - \alpha_+}{\alpha_+ + \alpha_-} \in (-1, 1)$ and omit multiplication of the metric by a constant factor as irrelevant, resulting in a single-parametric family of physical metrics. A comforting result of [38] furthermore establishes unitary equivalence of metrics with different α. This leaves us essentially with a unique physical inner product, realized e.g. by the natural choice $\alpha = 0$ as

$$(\phi, \psi)_\Theta = (\Phi, \Theta\Psi) = (\phi, D\psi) - (\dot{\phi}, \dot{\psi}) \tag{1.30}$$

Since D is unbounded on $L^2(\mathbb{R})$, the same holds for Θ for any α. This must be taken as a warning, since eq. 1.28 has to be understood as quasi-hermitian in a generalized sense, and possible pathologies may appear.

Probability current

The construction of the physical inner product for the Klein-Gordon equation may be seen as a first step to its quantum interpretation. The second complementary step would require constructing a positive and conserved probability density $\rho(x, t)$. The law of conservation amounts to

$$\partial_t \rho(x, t) + (\nabla j)(x, t) = 0 \tag{1.31}$$

for some vector $j(x, t)$. In another language, $\rho(x, t)$ must be a null component of a conserved four-vector. Consider, for example, the Schrödinger equation, which possesses a conserved current $j^\mu = (\rho, j)$ with the components

$$\rho = \psi\psi^* \qquad\qquad j = i(\psi^* \nabla\psi - \psi\nabla\psi^*) \tag{1.32}$$

Recalling that the usual inner product on the space of solutions of the Schrödinger equation is $(\phi, \psi) = \int \phi^* \psi$, it follows that the null probability density determines the inner product (or equivalently, the norm) through the relation $(\phi, \phi) = \int \rho(x, t) dx$. Moreover, $\rho = \psi\psi^*$ implies the existence of an inner product, which remains conserved in time

$$\begin{aligned}\frac{d}{dt}(\phi(t),\psi(t)) &= \frac{d}{dt}\int_{\mathbb{R}^3}\phi(x,t)\psi^*(x,t)\,dx = \\ &= \int_{\mathbb{R}^3}\frac{\partial\phi(x,t)}{\partial t}\psi(x,t) + \int_{\mathbb{R}^3}\phi(x,t)\frac{\partial\psi(x,t)}{\partial t} = \\ &= \int_{\mathbb{R}^3}\nabla\phi(x,t)\psi(x,t) + \int_{\mathbb{R}^3}\phi(x,t)\nabla\psi(x,t) = \int_{\mathbb{R}^3}\nabla(\phi\psi)(x,t) = 0\end{aligned} \tag{1.33}$$

In general, any probability density gives rise to a conserved inner product through analogous procedure. One such inner product for the Klein-Gordon equation was derived just in the last section. Here we shortly examine the possibility to work backwards and get a conserved probability density from a conserved inner product [37, 39]. The quantity usually known as the Klein-Gordon inner product

$$j^\mu = i(\psi^*\partial^\mu\psi - \psi\partial^\mu\psi^*) \tag{1.34}$$

fails to have a positive null component (despite being conserved in time), and thus cannot be used for our present purposes. However, inspired by the non-relativistic scenario, we might define the null component of the desired current to be the integrand of eq. 1.30

$$j^0_{KG} = \psi^* D\psi - \dot{\psi}^*\dot{\psi} \tag{1.35}$$

The remaining components of the four-current may then be found by performing an infinitesimal Lorentz boost on x and imposing the requirement of covariance on j^μ (details of this procedure may be found in [37], sec.2). The result is expressed compactly as $j^\mu = \psi^*\partial^\mu D\dot{\psi} - \partial^\mu\dot{\psi}^*\psi$, with the covariance as well as conservation of this final quantity to be verified directly from the definition.

1.2.2 The Proca equation

Equations governing the motion of relativistic particles can be organized into a well-known hierarchy according to the particle's spin (with first member of this hierarchy being the Klein-Gordon equation discussed above). The transformation into canonical form was successfully defined for several of these equations [40, 41], making them suitable for analysis with tools of quasi-hermitian theory. We start from the Dirac equation for particles of spin 1/2. This equation can not only be written in a Schrödinger-like form, but its most common expression $(i\gamma^\mu\partial_\mu - m)\psi = 0$ is actually of this type, using a 4×4 matrix Hamiltonian

$$H = \begin{pmatrix} m & & \partial_z & \partial_x + i\partial_y \\ & m & \partial_x - i\partial_y & -\partial_z \\ \partial_z & \partial_x + i\partial_y & -m & \\ \partial_x - i\partial_y & -\partial_z & & -m \end{pmatrix} \tag{1.36}$$

Note that this is just one particular (Dirac) representation of the gamma matrices appearing in the equation, other (equivalent) four-dimensional representations (Majorana, Newton-Wigner and others) may be also useful. Since the Dirac Hamiltonian is already hermitian *per se*, there

is no need to apply the machinery of quasi-hermitian theory. This is further demonstrated in the existence of a conserved four-current with a positive null component

$$j^\mu = \overline{\psi}\gamma^\mu\psi \tag{1.37}$$

where we define the Dirac adjoint $\overline{\psi} = \psi^\dagger\gamma^0$. Indeed, the null component of this four vector is $j^0 = \psi^\dagger\gamma^0\gamma^0\psi = \psi^\dagger\psi$, a manifestly positive quantity. Note that despite these promising features, there are further conceptual problems with single-particle Dirac equation, manifested for example by the Klein paradox [42].

Making one step up the hierarchy, one arrives at the Proca equation, which describes relativistic particles of spin 1, also called vector bosons [43]. It is commonly expressed using the four-potential A^μ as

$$\partial_\mu(\partial^\mu A^\nu - \partial^\nu A^\mu) + m^2 A^\nu = 0 \tag{1.38}$$

Every component of A^μ separately obeys the Klein-Gordon equation, with the components being tied together by an additional constraint $\partial_\mu A^\mu = 0$. Once again (and somewhat surprisingly), we may transform the Proca equation into the canonical form using a 6×6 matrix Hamiltonian. As long as we define the formal analogue of electric intensity $\vec{E} = \partial_t\vec{A} - i\nabla A^0$, we may write

$$H = \begin{pmatrix} & & & \partial_x^2 - m^2 & \partial_x\partial_y & \partial_x\partial_z \\ & & & \partial_y\partial_x & \partial_y^2 - m^2 & \partial_y\partial_z \\ & & & \partial_z\partial_x & \partial_z\partial_y & \partial_z^2 - m^2 \\ -\partial_x^2 - \omega^2 & -\partial_x\partial_y & -\partial_x\partial_z & & & \\ -\partial_y\partial_x & -\partial_y^2 - \omega^2 & -\partial_y\partial_z & & & \\ -\partial_z\partial_x & -\partial_z\partial_y & -\partial_z^2 - \omega^2 & & & \end{pmatrix} \qquad \Psi = \begin{pmatrix} m\vec{A} \\ i\vec{E} \end{pmatrix} \tag{1.39}$$

with $\omega^2 = \Delta + m^2$. This Hamiltonian may be in principle manipulated to obtain the general family of admissible inner products. A first step in this direction was made in [44] with a construction of a particular (positive) metric

$$\begin{pmatrix} m^2 - \partial_y^2 - \partial_z^2 & \partial_x\partial_y & \partial_x\partial_z & \alpha m\omega & & \\ \partial_x\partial_y & m^2 - \partial_x^2 - \partial_z^2 & \partial_y\partial_z & & \alpha m\omega & \\ \partial_x\partial_z & \partial_y\partial_z & m^2 - \partial_x^2 - \partial_y^2 & & & \alpha m\omega \\ \alpha m\omega & & & \omega^2 + \partial_y^2 + \partial_z^2 & -\partial_x\partial_y & -\partial_x\partial_z \\ & \alpha m\omega & & -\partial_x\partial_y & \omega^2 + \partial_x^2 + \partial_z^2 & -\partial_y\partial_z \\ & & \alpha m\omega & -\partial_x\partial_z & -\partial_y\partial_z & \omega^2 + \partial_x^2 + \partial_y^2 \end{pmatrix} \tag{1.40}$$

In addition, the importance of this metric was supported by establishing its Lorentz invariance, expressed by the condition $M^\dagger\Theta = \Theta M$ for an appropriate representation of Poincare algebra generators M. A more complete account regarding the construction of metrics for eq. 1.39 can be found in [45].

Quantization schemes

The quantization of the Proca equation is somewhat more involved than both the Dirac and the Klein-Gordon equations, since eq. 1.38 is a constrained system (only three components of A^μ are actual dynamical variables). A common approach in such case is to remove the auxiliary degrees of freedom *before* the quantization process itself. Writing the Lagrangian density corresponding to the Proca equation as

$$\mathcal{L} = m^2 A^*_\mu A^\mu - \frac{1}{2}\left(\partial_\mu A^*_\nu - \partial_\nu A^*_\mu\right)\left(\partial^\mu A^\nu - \partial^\nu A^\mu\right) \tag{1.41}$$

one readily sees that the null component of the canonical momentum satisfies $\pi_0 = \partial\mathcal{L}/\partial_{A_{0,t}} = 0$. Consequently, we might eliminate the null field components using $A_0 = (\partial_m \pi^*_m)/m^2$. After a straightforward calculation, the Hamiltonian density of the system is then expressed as

$$\mathcal{H} = \pi^*_m \pi_m + \frac{1}{m^2}\pi^*_{m,m}\pi_{n,n} + m^2 A^*_m A_m + A^*_{m,n}A_{n,m} - A^*_{m,m}A^*_{n,n} \tag{1.42}$$

showing that it is completely independent on A_0. Having successfully removed the nonphysical degrees of freedom, the quantization of this Hamiltonian may proceed in the usual canonical formalism. This is precisely the approach used to derive eq. 1.39, explaining also the six-dimensional nature of the result (instead of expected eight dimensions).

Alternatively, the constraint may be quantized together with the dynamics in the formalism of Dirac quantization [46]. This is the approach taken in [47], where three seemingly different but equivalent recipes are shown for quantizing the Proca system. In such case, the resulting canonical Hamiltonian has of course dimension eight.

Chapter 2

Solvability and computational aspects

2.1 Solvability and quasi-hermitian theory

We have seen that, despite providing a mere new mathematical formalism comparable e.g. to the Heisenberg or interaction pictures, quasi-hermitian theory leads to unexpected results concerning interpretation of relativistic wave equations. The usual application of the theory, however, is more modest: since nontrivial metrics allow in principle for a more general class of solvable operators, the aim is to search for such models and compute their spectra. *Pars pro toto*, we have included this review chapter devoted entirely to the concept of solvability in quantum mechanics as a whole [48].

Be warned, however, that the very notion of a solvable quantum operator is not unambiguous throughout the literature. It is often required, that the Schrödinger equation satisfies certain regularity conditions. Most of the commonly known potentials (among them the harmonic oscillator, hydrogen atom, Morse and Pöschl-Teller potentials) are solvable in this sense, with the corresponding Schrödinger equation belonging to the hypergeometric family. Interestingly, hypergeometric solvable potentials have been, after a long-lasting effort, described and classified completely [49, 50]. Classification of potentials corresponding to a more general Heun class of differential equations is currently in progress [51, 52].

2.1.1 Toeplitz matrices

Toeplitz matrices are probably the most general class of discrete models, which allows for general explicit formulas describing the spectrum [53]. They may be generally divided into four kinds. A finite Toeplitz matrix is any $n \times n$ matrix (a_{ij}) having constant diagonal entries, that is $a_{i,j} = a_{i-j}$. A Toeplitz matrix with entries wrapping around as $a_{k-n} = a_k$ is called a circulant matrix. Infinite-dimensional analogues of these matrices are defined as constant-diagonal matrices on $\ell^2(\mathbb{N})$ (infinite Toeplitz matrices), respectively $\ell^2(\mathbb{Z})$ (Laurent matrices). Note that the latter case already encompasses the circulant structure without additional requirements.

For infinite matrices, it is generally not clear whether they define a closed operator on ℓ^2, and what is such an operator's domain. However, as long as we restrict attention to bounded operators, a complete and simple characterization exists. Let's pick any orthonormal basis (ψ_n) of the underlying Hilbert space. An infinite Toeplitz (Laurent) matrix A then defines a

bounded operator on $\ell^2(\mathbb{N})$ or $\ell^2(\mathbb{Z})$ through the relation $a_{ij} = (\psi_i, A\psi_j)$, if and only if there is a function $a \in L^\infty(\mathbb{T})$, such that

$$a_n = \frac{1}{2\pi} \int_0^{2\pi} a(e^{i\theta}) e^{-in\theta} d\theta \tag{2.1}$$

where $\mathbb{T}$ denotes the unit circle. Moreover, the norm of such an operator is $\|A\| = \|a\|_\infty$ (see [53], thm. 1.1 and 1.9 for a proof). Since the correspondence between bounded Toeplitz operators and functions $a \in L^\infty(\mathbb{T})$ is one-to-one, the most common way of encoding information about the whole Toeplitz matrix is through its associated function

$$a(z) = \sum_{k=-\infty}^{\infty} a_k z^k \tag{2.2}$$

Every circulant and every Laurent matrix A is normal, since it may be written as a convolution operator $Av = a \star v$ for some vector a. Convolution operators are related to multiplication operators by Fourier transform, and all bounded multiplication operators are normal ([54], ex. 3.8). This is however not true for general Toeplitz matrices [55].

The general correspondence between A and $a(z)$ can be exploited to characterize the spectrum of A. In the following, we let $\mathbb{T}$ once again denote the unit circle, and $\mathbb{T}_n$ the set of n-th roots of unity. The most general theorem of this section allows to describe the spectrum of Laurent operators: it coincides with the essential range of the corresponding function.

$$\sigma(A) = \mathcal{R}(a) := \{\lambda \in \mathbb{C} \mid \mu(t \in \mathbb{R}, |a(t) - \lambda| < \varepsilon) > 0\} \tag{2.3}$$

with $\mu(\cdot)$ being the usual Lebesgue measure ([53], thm. 1.2). Note that the function $a(z)$ does not have to be differentiable or even continuous. In order to formulate the remaining theorems, we shall have to be more modest, and restrict attention to continuous symbols $a \in C(\mathbb{T})$. First, observe that for this kind of symbols, the formula above becomes $\sigma(A) = a(\mathbb{T})$. Additionally, we can describe the spectra of

- finite circulant matrices as $\sigma(H(a)) = a(\mathbb{T}_n)$
- infinite Toeplitz matrices as $\sigma(H(a)) = a(\mathbb{T})$ together with $\lambda \in \mathbb{C}$, such that $I(\lambda, a) \neq 0$.

with $I(a, \lambda)$ being the winding number of a around λ (see [53], thm. 1.17). In contrast, no simple characterization of eigenvalues exists for finite Toeplitz matrices. The closest one can get to the above theorems is a characterization of resolvent growth of such matrices with their growing dimension. This is most nicely formalized using the concept of pseudospectrum

$$\sigma_\varepsilon(H) = \left\{\lambda \in \mathbb{C} \mid \|(H - \lambda)^{-1}\| > \varepsilon^{-1}\right\} \tag{2.4}$$

which shall be discussed later in detail. To illustrate the behavior of finite Toeplitz matrices, fig. II shows a plot of the spectrum and pseudospectrum of a finite Toeplitz and finite circulant matrix of dimension 100 associated with the same function $a(z)$.

Despite the eigenvalues of the two matrices (black dots) being substantially different, the pseudospectral lines trace out exactly the same pattern in the complex plane. This is indeed a

(a) *finite Toeplitz matrix* (b) *finite circulant matrix*

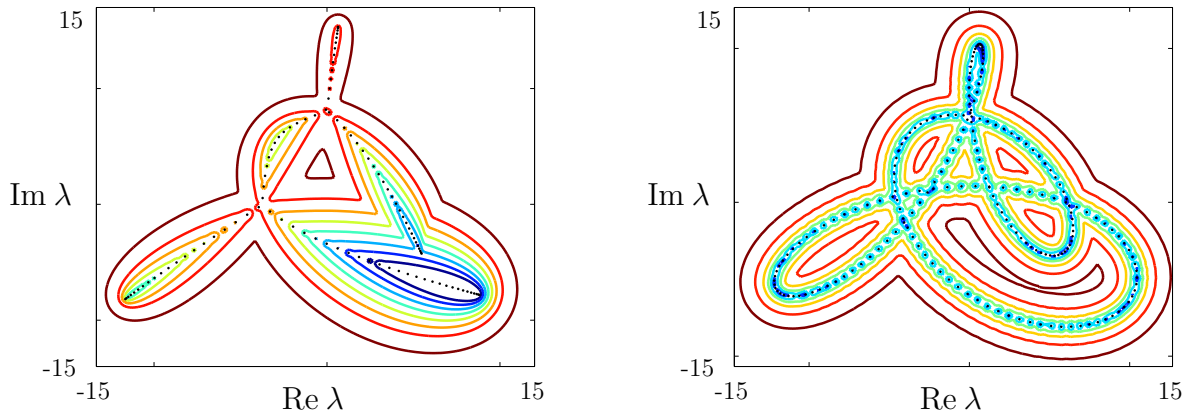

Figure II: *Spectra and pseudospectra corresponding to* $a(z) = \mathrm{i}z^{-3} - 5z^{-2} + 6z^{-1} - 3z^2 - 8\mathrm{i}z^3$

general property of finite Toeplitz matrices, which may be formalized into a theorem ([56], thm. 7.2). It states, that the resolvent norm $\|(A_n - \lambda)^{-1}\|$ of a sequence of finite Toeplitz matrices remains uniformly bounded whenever $I(a, \lambda) = 0$, but grows exponentially with n as long as $I(a, \lambda) \neq 0$ (at least for n sufficiently large), that is

$$\|(A_n - \lambda)^{-1}\| \geq e^{cn} \qquad \text{for some } \; c > 0 \tag{2.5}$$

In another language, the theorem provides a convergence relation between pseudospectra of a sequence of finite Toeplitz matrices A_n and corresponding infinite Toeplitz matrix A. In the appropriately defined distance of sets (which is discussed later in this chapter), it shows that $\sigma_\varepsilon(A_n) \to \sigma_\varepsilon(A)$ as $n \to \infty$. Note, that (as seen already from fig. II) such convergence theorem apparently does not apply for the spectrum.

2.1.2 Constant-coefficient differential operators

The theory of differential operators with constant coefficients does, somewhat surprisingly, parallel the theory of Toeplitz matrices very closely. Consequently, the spectrum of such operators can be described in a very compact way. This follows from a more general possibility of constructing isomorphism between (bounded) Toeplitz matrices and (unbounded) constant-coefficient differential operators, as well as their appropriate subclasses. The general differential operator with constant coefficients realizes itself as a formal expression

$$(A\psi)(x) = \sum_{j=0}^{d} a_j \psi^{(j)}(x) \tag{2.6}$$

where d is usually called the degree of the operator. Its domain must be defined appropriately, in order for the resulting operator to be closed. In our discussion, it is chosen as a subdomain of $AC^{d-1}(\mathbb{R})$, functions with absolutely continuous $(d-1)$-th derivative (in the special case

$d = \infty$, this means the functions have to be analytic). We again define a symbol uniquely determining each constant-coefficient differential operator

$$a(k) = \sum_{j=0}^{d} a_j (-ik)^j \tag{2.7}$$

which shall be used to elegantly describe its spectrum. We discuss four possible domains for eq. 2.6, which shall be revealed to correspond closely to the four classes of Toeplitz matrices. These domains and their discrete counterparts are summarized in tab. A (where the statement "β homogeneous boundary condition at x_0" means $\psi(x_0) = \psi'(x_0) = \cdots = \psi^{(\beta-1)}(x_0) = 0$).

domain of constant-coefficient differential operator	**Toeplitz matrix**
$AC^d(\mathbb{R})$	infinite Laurent
$AC^d[0,\kappa]$ with d periodic conditions	finite circulant
$AC^d(\mathbb{R}^+)$ with $\beta \leq d$ homogenous conditions at $x = 0$	infinite Toeplitz
$AC^d[0,\kappa]$ with β hom. cond. at $x = 0$ and γ hom. cond. at $x = \kappa$	finite Toeplitz

Table A: *Analogies between constant-coefficient differential operators and Toeplitz matrices.*

Compared to theorems formulated in the preceding section, there is an additional degree of freedom for two of these scenarios, manifested in the presence of parameters β and γ. We shall see that strict analogy applies as long as we choose $\beta = d$ and $\gamma = 0$. As for the first three cases, we can again formulate theorems characterizing the spectrum

- on $AC^d(\mathbb{R})$, we have $\sigma(A) = \mathcal{R}(a)$
- on $AC^d[0,\kappa]$ with d periodic conditions, we have $\sigma(A) = a(2\pi\mathbb{Z}/\kappa)$
- on $AC^d(\mathbb{R}^+)$ with β homogenous conditions at $x = 0$, we have $\sigma(H) = a(\mathbb{R})$ together with all $\lambda \in \mathbb{C}$ satisfying $I(a,\lambda) \neq d - \beta$

where the statement on $AC^d(\mathbb{R})$ holds for any $a \in L^\infty(\mathbb{T})$, whereas the remaining ones require $a \in C(\mathbb{T})$. The role of finite Toeplitz matrices is played by operators on a finite interval with homogeneous conditions at both ends. Again, we might employ more general conditions, and assume that there are β conditions at $x = 0$ and γ conditions at $x = \kappa$. Then the theorem concerting growth of the resolvent function states, that

$$\|(A_\kappa - \lambda)^{-1}\| \geq e^{c\kappa} \qquad \text{for some } \; c > 0 \tag{2.8}$$

whenever $I(a,\lambda) < d - \beta$ or $I(a,\lambda) > \gamma$ (see [56], thm. 10.2). Note that for $\gamma = d - \beta$, this condition becomes $I(a,\lambda) \neq d - \beta$. For these more restricted boundary condition, the above statement might be again reformulated in terms of pseudospectral convergence, $\sigma_\varepsilon(A_\kappa) \to \sigma_\varepsilon(A)$ as $\kappa \to 0$, where A acts on the half-line with β conditions at zero.

Convection-diffusion operator

Differential operators (including those with constant coefficients) appear, unlike Toeplitz matrices, ubiquitously in almost all areas of physics. One such operator serves in fluid mechanics, semiconductor physics are related areas to to describe the transfer of particles or energy due to combination of two processes: convection and diffusion [57]. Such operator has to be non-hermitian by definition (since diffusion is a non-reversible, and therefore non-unitary process), The simplest reasonable choice is

$$(H\psi)(x) = -\psi''(x) + \psi'(x) \tag{2.9}$$

We consider this operator on two domains: the whole real line, and a finite interval $[0, \kappa]$ with $\beta = \gamma = 1$ (corresponding to fixed ends of a string, or impenetrable walls). On the first of those domains, the spectrum may be readily written down as the range of $a(z) = -iz - z^2$, which is a parabola in the complex plane

$$\sigma(H) = \left\{\lambda \in \mathbb{C} \mid (\operatorname{Im}\lambda)^2 = \operatorname{Re}\lambda\right\} \tag{2.10}$$

On $[0, \kappa]$, the spectrum cannot be characterized with the help of above theorems, it can be however computed by hand using a simple trick. Let's consider a transformation $\Omega = \exp(x/2)$, and observe that the convection-diffusion Hamiltonian is similar to a hermitian operator

$$(H'\psi)(x) = (\Omega H \Omega^{-1}\psi)(x) = -\frac{1}{4}\psi(x) + \psi''(x) \tag{2.11}$$

defined on the same domain. This similarity transformation is bounded and nonsingular for any $\kappa < \infty$, making H and H' isospectral. The eigenvalue equation for H' may be solved exactly, with the result

$$\sigma(H') = \left\{-\frac{1}{4} - \frac{\pi^2 n^2}{\kappa^2} \;\middle|\; n \in \mathbb{N}\right\} \tag{2.12}$$

This reasoning however breaks down for $\kappa = \infty$. The formal similarity of the two differential operators no longer guarantees their isospectrality, and indeed, their spectra are substantially different. While the spectrum of H, as we have seen, forms a parabola in the complex plane, the spectrum of H' is a real half-line $(-1/4, \infty)$. Both spectra together with contours of the resolvent are shown in fig. III.

2.1.3 Solvability and supersymmetry

Supersymmetry, in its original setting, is a theory describing a suggested type of spacetime symmetry between bosons and fermions [58, 59]. In a theory with unbroken supersymmetry, any boson would have its supersymmetric fermion partner with the same mass, charge etc, differing only by its spin. This is naturally not observable in our universe, meaning that an actual existing supersymmetry would have to be spontaneously broken. Its existence is still a matter of discussion, both theoretical and phenomenological.

The ideas of supersymmetry may be applied to quantum mechanics, where they closely relate to the concept of solvability [60, 61], and extend the factorization method proposed

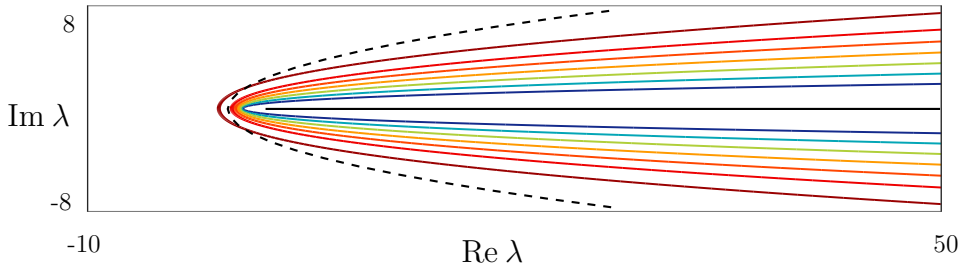

Figure III: *Spectra and resolvent contours of eq. 2.9 (solid and colored lines), together with the spectrum of eq. 2.11 (dashed lines). While the spectra of the two models may be substantially different, the resemblance of the pseudospectra is undisputed.*

initially by Infeld and Hull [62]. Instead of bosons and fermions, the objects of interest are two Hamiltonians with potentials $V_1(x)$ and $V_2(x)$, intertwined in terms of a so-called superpotential $W(x)$. From the knowledge of this superpotential, we may define the creation and annihilation operators as

$$\begin{aligned}(a\psi)(x) &= \psi'(x) + W(x)\psi(x)\\ (a^\dagger\psi)(x) &= -\psi'(x) + W(x)\psi(x)\end{aligned} \tag{2.13}$$

The partner Hamiltonians may then be written as $H_1 = a^\dagger a$ and $H_2 = aa^\dagger$ (by definition, both of these operators are positive). In terms of the superpotential, this means that the partner potentials can be expressed as $V_{1,2}(x) = W^2(x) \pm W'(x)$. The corresponding Hamiltonians are then related in terms of eigenvalues, eigenfunctions, and scattering data. Indeed, assume that $H_1\psi = aa^\dagger\psi = E_n\psi$. Then

$$H_2(a\psi) = aa^\dagger a\psi = aH_1\psi = E(a\psi) \tag{2.14}$$

and we have constructed an eigenstate of H_2 from the eigenstate of H_1, corresponding to the same energy. For operators with discrete spectrum, this means that H_1 and H_2 are isospectral, unless $A\psi = 0$. If this happens, H_1 has zero ground energy and $\psi(x)$ is the corresponding (nodeless) ground state. This is a very special case in supersymmetric quantum mechanics, a so-called unbroken supersymmetry. In this precise scenario, we might explicitly write $W(x)$, and consequently $H_2(x)$, merely from the knowledge from the ground state $\psi_0(x)$ of H_1 as

$$W(x) = \frac{\psi_0'(x)}{\psi_0(x)} \tag{2.15}$$

The Hamiltonian H_2 constructed through this procedure is being isospectral to H_1, with the exception of the lowest eigenvalue. This has important theoretical consequences in case the spectrum of H_1 can be evaluated explicitly. In particular, we might readily write down the whole spectrum of the newly constructed Hamiltonian using merely the knowledge of spectrum of H_1 and its ground state.

Up to now, we have used supersymmetry to construct new potentials from known, possibly solvable, ones. However, supersymmetric techniques can be also used to construct spectra of

certain Hamiltonians *per se*. For this to happen, it suffices that the partner potential differs from the original one only by an inessential change of parameters. This is formalized in the condition of shape-invariance

$$V_2(x, a_1) = V_1(x, a_2) + R(a_1) \tag{2.16}$$

Here $a_2 = f(a_1)$ is supposed to be a certain well-behaved function of a_1, and the same applies for $R(a_1)$. To prove this assertion, we use the shape-invariance condition repeatedly to construct an infinite hierarchy of Hamiltonians H_n. Inserting eq. 2.16 into the p-th and the $p+1$-th Hamiltonians results in

$$\begin{aligned}(H_p\psi)(x) &= -\psi''(x) + V_1(x, a_p)\psi(x) + \sum_{k=1}^{p-1} R(a_k)\psi(x) \\ (H_{p+1}\psi)(x) &= -\psi''(x) + V_1(x, a_{p+1})\psi(x) + \sum_{k=1}^{p} R(a_k)\psi(x)\end{aligned} \tag{2.17}$$

Since these two Hamiltonians are supersymmetric partners, they necessarily have the same spectrum except for the zero ground state of H_p. Going back down the hierarchy to $p = 0$ and using the isospectrality condition, we arrive to the expression for the n-th eigenvalue of H_1

$$E_n^{(1)} = E_0^{(n)} = \sum_{k=1}^{n} R(a_k) \tag{2.18}$$

Almost all known analytically solvable potentials are shape invariant in this sense. As an example, consider the radial Coulomb and harmonic oscillator potentials indexed by their discrete angular momentum ℓ, which shall naturally take the role of the auxiliary parameter in eq. 2.16. The shape invariance conditions for both these potentials are then

$$\begin{aligned} V_l(r) &= \frac{l(l+1)}{r^2} + \frac{e}{r} & V_2(r, l, e) &= V_1(r, l+1, e) + \left[\frac{e^4}{4(l+1)^2} - \frac{e^4}{4(l+2)^2}\right] \\ V_l(r) &= \frac{l(l+1)}{r^2} + \omega^2 r^2 & V_2(r, l, \omega) &= V_1(r, l+1, \omega) - (l+1/2)\omega + (l+5/2) \end{aligned} \tag{2.19}$$

which, together with eq. 2.18, result in the well-known expressions for their eigenvalues without need of solving any differential equation.

Finally, we comment shortly about the relation between the supersymmetry used in this section and actual supersymmetry in particle physics. Although both concepts look substantially different at first sight, they share the algebraic structure of a superalgebra $\mathfrak{sl}(1,1)$. This superalgebra arises in our context through the following entities defined in terms of the Hamiltonian and the ladder operators

$$H = \begin{bmatrix} H_1 & 0 \\ 0 & H_2 \end{bmatrix} \qquad Q = \begin{bmatrix} 0 & 0 \\ a & 0 \end{bmatrix} \qquad Q^\dagger = \begin{bmatrix} 0 & a^\dagger \\ 0 & 0 \end{bmatrix} \tag{2.20}$$

Computing their (anti)-commutation relations indeed reveals the structure of $\mathfrak{sl}(1,1)$, which is a $\mathbb{Z}_2$ graded algebra admitting decomposition into even and odd elements, such that the algebra multiplication respects the grading.

$$\begin{gathered}[H,Q] = [H^\dagger, Q^\dagger] = 0 \qquad\qquad \{Q, Q^\dagger\} = H \\ \{Q,Q\} = \{Q^\dagger, Q^\dagger\} = 0\end{gathered} \tag{2.21}$$

Examples

The supersymmetric machinery outlined above may be applied iteratively, using the newly constructed Hamiltonian H_2 as a new starting point. This way, we arrive in principle at an infinite hierarchy of Hamiltonians with closely related spectral properties. As an example, let H_1 be a Hamiltonian of the infinite square well on $[0,\kappa]$ with

$$V(x) = \begin{cases} 0 & \text{for } x \in [0,\kappa] \\ +\infty & \text{otherwise} \end{cases} \tag{2.22}$$

Its spectrum can be evaluated directly to be $E_n = \pi^2(n+1)^2/\kappa^2$. We subtract its ground state energy $E_0 = \pi^2/\kappa^2$ by redefining $H \to H - E_0$ in order to reach the state of unbroken supersymmetry (otherwise, we shall not be able to express the partner Hamiltonian explicitly). After evaluating H_2, we might repeat this algorithm any number of times, obtaining a hierarchy of Hamiltonians indexed by a discrete parameter p

$$V_{p+1}(x) = \frac{\pi^2 p(p+1)}{\kappa^2} \csc^2\left(\frac{\pi x}{\kappa}\right) \tag{2.23}$$

By construction, the spectrum of these operators may be readily determined without further computations as $E_n^{(p+1)} = \frac{\pi^2}{\kappa^2}\{n(n+2p+2)+p^2\}$. The fact, that potentials with $p \geq 1$ are essentially equivalent to each other up to a change of parameters, is a clear demonstration of their shape invariance. On the other hand, the square well itself is substantially different in shape from this family, as demonstrated in fig. IV.

Figure IV: *Low lying eigenstates of the square potential well (left) as well as the first member of eq. 2.23 (right). The first excited state of the square well corresponds to the ground state of the second potential.*

The technique of supersymmetry can be also applied to Hamiltonians with continuous spectra, and used to relate their scattering matrices. In order to proceed, we define $W_\pm = W(x = \pm\infty)$.

Then, in a way outlined in [60], we may relate the reflection and transmission coefficients of the partner Hamiltonians as

$$R_1(k) = \left(\frac{W_- + ik}{W_- - ik}\right) R_2(k) \qquad T_1(k) = \left(\frac{W_+ - ik'}{W_- - ik}\right) T_2(k) \tag{2.24}$$

with $k^2 = E - W_-^2$ and $k'^2 = E - W_+^2$. From this relation, we can deduce that $|R_1(k)|^2 = |R_2(k)|^2$ and $|T_1(k)|^2 = |T_2(k)|^2$; the partner potentials have identical reflection and transmission coefficients. As an example, we shall construct a hierarchy of supersymmetric partners corresponding to the free particle. Consider a free particle potential, chosen as $V(x) = \alpha^2/2$. Its superpotential may be readily computed as a solution of the equation $W^2(x) - W'(x) = V(x)$, which is $W(x) = \alpha \tanh(\alpha x)$. The corresponding hierarchy of p-indexed potentials is

$$V_{p+1}(x) = \frac{\alpha p(p+1)}{\cosh^2(\alpha x)} - p^2 \tag{2.25}$$

with the p-th potential having precisely p bound states and a band of continuous spectrum. By construction, this family of potentials is reflectionless, which is often a desired property in applications, as for example in theoretical realizations of invisibility [63].

2.2 Numerical issues

In contrast to the wealth of available analytic methods, the class of solvable Hamiltonians is usually too narrow to serve the practical needs of physical experiments. Numerical methods must be used to examine the majority of phenomenologically relevant operators, and it is thus crucial to understand the questions of applicability and convergence of such methods. Consequently, we complement the discussion of analytic methods by its numerical counterpart, with the choice of methods reflecting our focus on analysis of non-hermitian operators.

2.2.1 Pseudospectrum

One of the most fundamental results in the theory of normal operators is the spectral theorem. Its essence lies in the fact, that any normal (and thus also any hermitian) operator may be completely described from the knowledge of its spectrum (including degeneracies). Since the spectrum is a simple and nicely visualized concept, it often provides a more convenient description of the system than the elusive entity of a Hilbert space operator.

For non-normal operators, the spectral theorem does not hold, and the spectrum is no longer sufficient to encode complete information about their behavior. When performing non-normal analysis, one has to look at other quantities in order to obtain the desired knowledge about the operators. Since the spectrum consists of poles of the resolvent function, a logical step would be to take a closer look at the resolvent function itself, and in particular its norm. This is the essential idea behind the definition of the pseudospectrum

$$\sigma_\varepsilon(H) = \left\{\lambda \in \mathbb{C} \mid \|(H-\lambda)^{-1}\| > \varepsilon^{-1}\right\} \tag{2.26}$$

where we tacitly assume that $\|(H-\lambda)^{-1}\| = \infty$ for $\lambda \in \sigma(H)$. We shall see shortly, that this notion is indeed trivial for normal operators, but can be highly nontrivial in general. Instead of the resolvent norm, the pseudospectrum may be described also in several other ways, three of which are listed below (see thm. 4.3 in [56] for a proof)

$$\begin{aligned}\sigma_\varepsilon(H) &= \{\lambda \in \mathbb{C} \mid \|(H-\lambda)v\| \leq \varepsilon, \|v\| = 1\} = \\ &= \{\lambda \in \mathbb{C} \mid \sigma_{min}(H-\lambda) \leq \varepsilon\} = \\ &= \{\lambda \in \mathbb{C} \mid \lambda \in \sigma(H+A), \|A\| < \varepsilon\}\end{aligned} \tag{2.27}$$

The vector v appearing in the first of these definitions is usually called a pseudoeigenvector. Its existence for every $\lambda \in \sigma_\varepsilon(H)$ shows, that the pseudospectrum coincides with the set of pseudoeigenvalues, and has no "continuous" and "residual" parts. The definition in terms of the lowest singular value $\sigma_{\min}$ is most suitable for doing numerical computations. Alternatively, one can use the last definition of eq. 2.27 to plot eigenvalues of perturbed Hamiltonians, producing a similar result. We show the results of both these methods in fig. V.

(a) *contour plot of the lowest singular value* (b) *eigenvalues of* 50 *random perturbations*

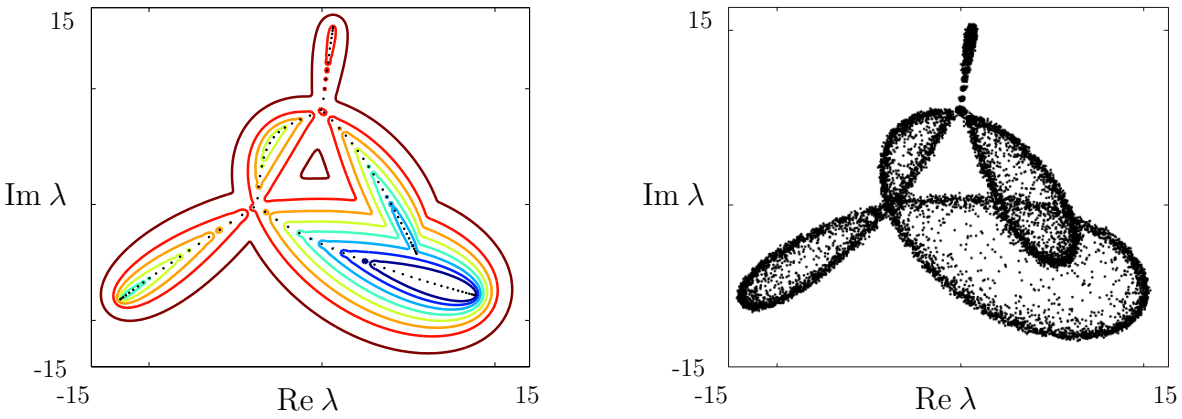

Figure V: *Pseudospectra taken from fig. II computed using two different numerical methods of eq. 2.27.*

The pseudospectrum of a normal operator behaves in a surprisingly trivial way. To see this, denote the ε-neighborhood of a set M in the usual Euclidean metric as $\Delta_\varepsilon(M)$. Next, recall that as a simple consequence of the spectral theorem, normal operator are diagonalizable by unitary transformations, that is $H = U^\dagger D U$. Making use of this fact, we may write

$$\begin{aligned}\|(H-\lambda)^{-1}\| &= \|(U^\dagger D U - \lambda U^\dagger U)^{-1}\| = \\ &= \|(D-\lambda)^{-1}\| = \rho(\lambda, \sigma(D))^{-1} = \rho(\lambda, \sigma(H))^{-1}\end{aligned} \tag{2.28}$$

which shows that $\sigma_\varepsilon(H) = \Delta_\varepsilon(\sigma(H))$ for any normal operator: the pseudospectrum is simply the ε-neighborhood of the spectrum. This has a direct consequence for quasi-hermitian operators.

Since any such operator H may be written as $H = \Omega^{-1} h \Omega$ for h hermitian, it follows directly from the definition, that

$$\sigma_\varepsilon(H) \subseteq \Delta_{\kappa(\Omega)\varepsilon}(\sigma(H)) \qquad \text{with} \qquad \kappa(\Omega) = \|\Omega\|\|\Omega^{-1}\| \tag{2.29}$$

(see also [56], thm. 3.4). When complemented by the inequality $\Delta_\varepsilon(\sigma(H)) \subseteq \sigma_\varepsilon(H)$ valid for any operator whatsoever, this imposes (non-sharp) bounds for ε-pseudospectrum of quasi-hermitian operators. This has an important consequence; a quasi-hermitian operator admitting a bounded and non-singular metric has its pseudospectrum confined to bounded region around $\sigma(H)$. Looking at a pseudospetral plot with contours escaping to infinity thus provides a strong indication for the nonexistence of a genuine metric. This behavior is illustrated in fig. VI for the imaginary cubic and harmonic oscillators.

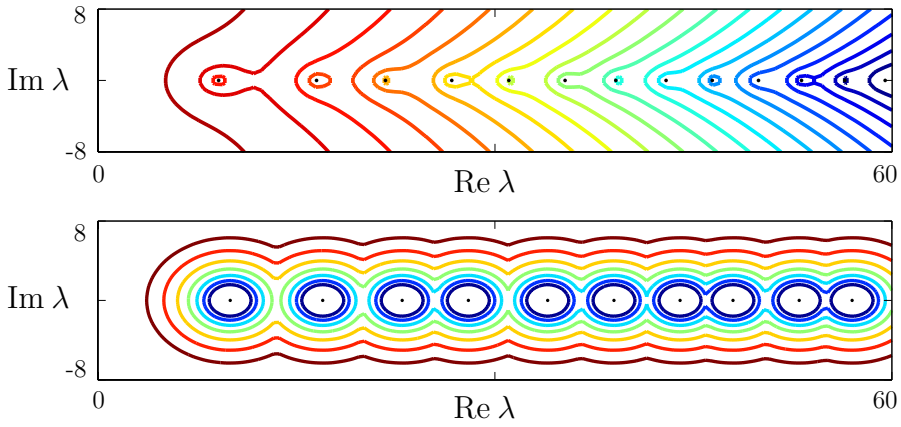

Figure VI: *Pseudospectra of the imaginary cubic oscillator (upper image) and the linear harmonic oscillator (lower image). The unbounded pseudospectra in the first plot have important consequences, which are discussed below.*

As we have seen already for Toeplitz matrices and constant-coefficient differential operators, the spectrum of a convergent operator sequence may behave quite unpredictably, while the pseudospectrum converges reasonably to its proper limit. This is indeed a general feature of the pseudospectrum. In order to formalize it, we must establish the notion of set convergence, most naturally defined in terms of the Hausdorff distance

$$\rho(M,N) = \max\left\{ \sup_{x\in M} \inf_{y\in N} \rho(x,y), \sup_{y\in N} \inf_{x\in M} \rho(x,y) \right\} \tag{2.30}$$

with $\rho(x,y)$ denoting usual Euclidean notion of distance. The notion of operator convergence may be defined in several ways, the most useful being norm convergence (applicable for bounded operators) and norm resolvent convergence (for unbounded operators with bounded resolvent). A natural generalization of both these notions is formalized in convergence under the so-called gap measure $\delta(H_1, H_2)$, see [64], sec. IV.2.

Using this notion enables us to state the convergence theorem in its most general form, taken from [65], thm 5.3. In addition to the assumed convergence in the gap measure $\hat{\delta}(H_n, H) \to 0$, we have to impose a somewhat technical condition, that $\|(H-\lambda)^{-1}\|$ is not constant on any

open set [66]. Then for each $\varepsilon > 0$ and each compact $K \subset \mathbb{C}$ such that $K^o \cap \sigma_\varepsilon(H) \neq 0$, the pseudospectra converge in the Hausdorff measure as

$$\rho\left\{\overline{\sigma_\varepsilon(H_n)} \cap K, \overline{\sigma_\varepsilon(H)} \cap K\right\} \to 0 \tag{2.31}$$

Semiclassical pseudospectrum

Since having an unbounded ε-pseudospectrum disproves the existence of a bounded and nonsingular metric, it could be in principle used to obtain rigorous proofs for such nonexistence, establishing important no-go theorems in the spirit of [28]. The only problem is, that the pseudospectrum may not be expressed in a closed form even for the simplest non-hermitian operators. This problem is often remedied using semiclassical pseudospectrum.

The notion of semiclassical pseudospectrum arose from theory of semiclassical differential operators in the works of Zworski and Davies [67, 68]. By a semiclassical differential operator, we understand an operator made dependent on an auxiliary parameter h as

$$(H_h\psi)(x) = \sum a_j(x) h^j \psi^{(j)}(x) \tag{2.32}$$

In complete analogy with eq. 2.7, we define the associated symbol for such an operator (which may now have possibly non-constant coefficients) as $a(x,\xi) = \sum a_j(x)(-i\xi)^j$. The semiclassical pseudospectrum is then a subset of complex plane defined as the closure of

$$\Lambda = \left\{ a(x,\xi) \;\middle|\; (x,\xi) \in \mathbb{R}^2, \frac{1}{2i}\left\{a, a^*\right\}(x,\xi) > 0 \right\} \tag{2.33}$$

with $\{a, a^*\}$ being the usual Poisson bracket. If we assume that our Hamiltonian is a Schrödinger operator with complex analytic potential $V(x)$, the associated symbol becomes $a(x,\xi) = -\xi^2 + V(x)$ and the above definition reduces to

$$\Lambda = \left\{\xi^2 + V(x) \mid \xi \in \mathbb{R}, \xi \operatorname{Im} V'(x) < 0\right\} \tag{2.34}$$

The importance of semiclassical pseudospectrum stems from a result concerning resolvent growth inside Λ in the classical limit $h \to 0$ (see [68], thm. 1). Its essential statement is, that for any $\lambda \in \Lambda$ exists some $c > 1$, such that $z \in \sigma_\varepsilon(H_h)$ for $\varepsilon \geq c^{-1/h}$. Consequently, for a given Hamiltonian, the semiclassical pseudospectrum lies inside the ε-pseudospectrum for sufficiently large values of ε.

This statement might be extended to non-semiclassical operators using the correspondence between the semiclassical limit $h \to 0$ and the high energy limit. For illustration of this procedure, we select again the imaginary cubic oscillator. Following [69], we transform it into a semiclassical operator for the purposes of the above theorem. If we define an unitary operator

$$(U\psi)(x) = \tau^{1/2}\psi(\tau x) \tag{2.35}$$

with $h = \tau^{-5/2}$, the transformation $UHU^\dagger = \tau^3 H_h$ results in the cubic oscillator in its semiclassical form $H_h = -h^2\Delta + ix^3$. Since unitary transformations leave the pseudospectrum unchanged, we have $\sigma_\varepsilon(H) = \tau^3\sigma_\varepsilon(H_h)$. The interior of semiclassical pseudospectrum of H_h

may be computed directly as $\Lambda = \{\lambda \in \mathbb{C} \mid \operatorname{Re}\lambda > 0, \operatorname{Im}\lambda \neq 0\}$. When performing the inverse transformation with $U^\dagger$, one has to make certain estimates in order to proceed [69, 70]. The final result may be established in the form of a set inclusion

$$\left\{ z \in \mathbb{C} \;\middle|\; |\arg z| < \frac{\pi}{2} - \delta, |z| \geq \max\left\{ c_1, c_2 \left(\log \varepsilon\right)^{6/5} \right\} \right\} \subseteq \sigma_\varepsilon(H)$$

in the sense, that for each $\delta > 0$ exist $c_{1,2}$ satisfying the inclusion. It is readily seen, that such set extends infinitely far into right complex half-plane for any δ, clearly demonstrating the nonexistence of a bounded nonsingular metric. The boundaries of this set for various values of ε are, together with boundaries of actual pseudospectra, shown in fig. VII.

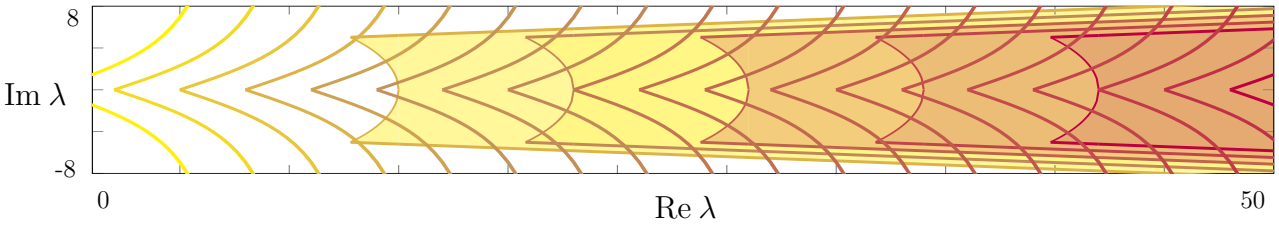

Figure VII: *Imaginary cubic oscillator; scheme of actual pseudospectra (thick lines) together with the sets defined in eq. 2.2.1 (filled) for multiple values of ε.*

2.2.2 Discretization of differential operators

Numerical methods for solving (ordinary or partial) differential equations for a given initial or boundary conditions are plentiful and well-developed. However, as long as we wish to obtain a complete solution not tied down to particular initial conditions, these is often no help coming from numerical analysis. For linear differential equations (where the knowledge of the complete solution equals the knowledge of the corresponding operator spectrum), we can however try to discretize the differential operator. The result of such operation would be a matrix of large dimension and, hopefully, similar spectral properties

Virtually all differential operators encountered in quantum theory are Schrödinger operators with local potentials $V(x)$, the discretization of which is trivial. Consequently, the problem of discretization degenerates basically into discretizing the operator of n-th derivative on various domains, subject to various boundary conditions (for further references on this topic, see [71] and [56], IX.43).

Basic method: finite differences

The most commonly encountered method for treating differential equations numerically is the method of finite differences. This method works on a regular discrete grid, which we shall take to be a one-dimensional equidistant set of points $\{x_0, \ldots, x_n\}$. Its essence lies in interpolating a chosen vector $\{u_0, \ldots, u_n\}$ by values of a certain polynomial on the grid, and evaluate its derivative at the nodes. The interpolation occurs locally, by choosing a different polynomial for each respective node.

Finite-difference methods are characterized by their order, corresponding to the order of interpolating polynomials. The lowest applicable order is $n = 2$. In such case, given a vector $\{u_0, \ldots, u_n\}$, we define a class of (uniquelly determined) degree 2 polynomials $p_j(x)$, such that $p_j(x_{j-1}) = u_{j-1}$, $p_j(x_j) = u_j$ and $p_j(x_{j+1}) = u_{j+1}$. Setting $D_{ij}u_j = p_i'(x_i)$ results in the expression for the differentiation matrix, shown for $n = 4$ as

$$D_{ij} = \frac{1}{2}\begin{bmatrix} -1 & & & & \\ 1 & -1 & & & \\ & 1 & -1 & & \\ & & 1 & -1 & \\ & & & 1 & \end{bmatrix} \tag{2.36}$$

Finite difference methods of higher order may be defined analogically; a method of order n uses polynomials of degree n interpolating $n + 1$ adjacent nodes. All these methods result in banded Toeplitz differentiation matrices with increasing number of diagonals. In the following, we are going to discuss methods of spectral discretization, which aim to take this process into the limit (resulting in non-banded, dense matrices). These methods often perform in orders of accuracy better than finite difference methods.

Periodic domains: Fourier interpolation

On periodic domains, we may use another method of interpolation, taking inspiration from Fourier analysis. It this case, the interpolants shall be global (ranging over the whole interval). It should come as no surprise, that they shall emerge as trigonometric polynomials (that is, polynomials in terms of $\sin(x)$ and $\cos(x)$). We take our domain to be a one-dimensional circle, or equivalently an interval $[0, 2\pi]$ equipped with periodic boundary conditions. We discretize the domain equidistantly, resulting in the nodes

$$x_j = \frac{2\pi j}{n} \tag{2.37}$$

In order to obtain the desired interpolating polynomial $p(x)$, we apply the discrete Fourier transform twice on a given vector (v_k). The first application results in $\tilde{v}_k = 2\pi/n \sum_{j=1}^{n} e^{-ikx_j} v_j$, while the second one, not constrained to discrete values of x_j, provides the desired interpolant

$$p(x) = \frac{1}{2\pi} \sum_{-n/2}^{n/2} e^{ikx} \tilde{v}_k \tag{2.38}$$

Taking into account our assumption of equidistant grid, this interpolant may be computed in a closed form ([71], sec. 3). As long as we write $p(x) = \sum_{k=1}^{n} v_k S_n(x - x_k)$, the quantity S_n (which is essentially the interpolant of a δ-function) may be expressed as

$$S_n(x) = \frac{\sin(nx/2)}{n \tan(x/2)} \tag{2.39}$$

This quantity encompasses complete information about differentiation matrices of arbitrary order. The resulting matrices are again circulant and Toeplitz, they are however no longer banded. As an example, the matrix expressing first derivative may be written as

$$D_{i-j} = S_n'(x_{i-j}) = \begin{cases} \frac{1}{2}(-1)^{j-i+1} \cot\left(\frac{(j-i)\pi}{n}\right) & \text{for } j \neq i \\ 0 & \text{for } j = i \end{cases} \tag{2.40}$$

Note that this matrix still remains anti-hermitian, an expected property of the derivative operator. Differentiation matrices of higher order may be constructed analogically.

Nonperiodic domains: orthogonal polynomials

For operators on non-periodic domains, the Fourier analysis approach is no longer applicable, and the interpolants have to be chosen as common (non-trigonometric) polynomials. However, it turns out we might get substantially more precise numerical methods by using global interpolants *and* modifying the underlying grid, so that the points are no longer equidistant. In particular, the grid might be chosen as the set of roots of some orthogonal polynomial. For simplicity, we discuss here the case of a bounded interval, and use the Chebyshev polynomials throughout this section. The Chebyshev nodes, clustering towards the boundaries of the interval, admit a closed-form expression

$$x_j = \cos\left(\frac{j\pi}{n}\right) \tag{2.41}$$

The rest of the construction algorithm proceeds in complete analogy with the method of finite differences. We take $p(x)$ to be the unique degree n polynomials interpolating a selected vector (v_n), and set $p'(x_j) = D_{ij}v_j$, with D_{ij} being the discretization matrix. The result is now neither anti-hermitian, nor Toeplitz. Still, its elements may be expressed through a sufficiently simple formula, as shown in fig. VIII (for derivation, see [71], ex. 6.1).

$$D_{ij}^{(n)} = \begin{array}{|c|c|c|} \hline \frac{2n^2+1}{6} & \frac{2(-1)^j}{1-x_j} & \frac{(-1)^n}{2} \\ \hline -\frac{(-1)^i}{2(1-x_i)} & \begin{array}{c} -\frac{(-1)^i}{2(1-x_i)} \\ \frac{-x_j}{2(1-x_j^2)} \\ -\frac{(-1)^i}{2(1-x_i)} \end{array} & \frac{(-1)^{n+i}}{2(1+x_i)} \\ \hline -\frac{(-1)^n}{2} & -\frac{2(-1)^{n+j}}{1+x_j} & -\frac{2n^2+1}{6} \\ \hline \end{array}$$

Figure VIII: *The $n \times n$ differentiation matrix arising from the Chebyshev interpolation method. The inner square is a $(n-2) \times (n-2)$ matrix, while the remaining boxes are scalars and $(n-2)$-dimensional vectors.*

For bounded intervals, the need of imposing some kind of boundary conditions often arises at the ends of the interval. The effect of those conditions on discretized operators is a delicate subject, with little to none generally applicable procedures. However, the probably most encountered

case - homogeneous conditions at the boundary - is known to be very faithfully represented by stripping the first and last rows and columns of the matrix (see [71], sec. 13).

In principle, one can construct a variety of discretization methods using any series of orthogonal polynomials. The choice of particular polynomial family is a matter of taste and experience, the only requirement being that the domain of the polynomials coincides with the domain of the operator to be discretized. As an example, for discretization of operators acting on the real half-line $(0, \infty)$, a convenient choice of grid points is the set of roots of a n-th order Laguerre polynomial [72].

Chapter 3

Applications to simple differential models

Quasi-hermitian theory may be seen as conceptually well understood, applying its machinery to differential Schrödinger operators however raises several problems, which are difficult to overcome. The biggest hindrance appears to be the non-locality of the physical hermitian partners corresponding to those operators [73]. On the other hand, the proper treatment of quasi-hermitian Schrödinger operators is absolutely essential for the future success of the theory, making it probably the primary subject of the field.

In this section, we address two simple examples of differential non-hermitian Hamiltonians, which correspond to two basic schemes for construction of such operators. While the first example appears as a result of quantizing a classical system with dissipative and nonconservative forces, the other one arises by a direct coupling modification of an originally hermitian quantum Hamiltonian.

3.1 Branched Hamiltonians

This section, inspired directly by [10], intends to provide some basic insight into the theory of classical multi-valued Hamiltonians and their quantization. In order to discuss properties of multi-valued Hamiltonians, we start from the field of classical physics, making all the Lagrangians and Hamiltonians of this section (configuration-space or phase-space) functions instead of Hilbert space operators.

The appearance of multi-valued Hamiltonians in classical physics can have at least two origins. They can be either Legendre transformed Lagrangians whose velocity dependence is not convex, in particular Lagrangians depending on the velocity more than quadratically [74, 75, 76, 77]. Alternativelly, they may also arise as continuous interpolations of certain discrete (e.g. chaotic) dynamical systems [78, 79]. As one of the simplest examples, consider the Lagrangian of [75]

$$L(x,\dot{x}) = \frac{\dot{x}^4}{4} - \frac{\kappa\dot{x}^2}{2} \tag{3.1}$$

The process of Legendre transforming this Lagrangian with respect to $\dot{x}$ is singular for $\kappa > 0$,

since the canonical momentum $p = \dot{x}^3 - \kappa x$ can have either one or three values of $\dot{x}$ for a given p. Consequently, the corresponding Hamiltonian is a multivalued function of momentum, as illustrated by the energy-momentum graph in fig. IX.

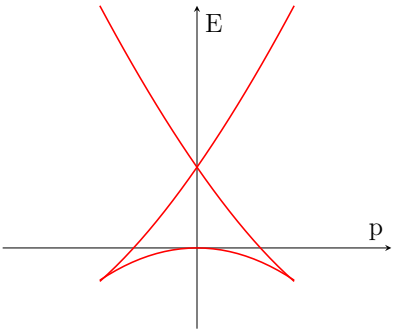

Figure IX: *The relationship between energy and momentum of eq. 3.1 as a multivalued function in the $E - p$ plane.*

More complicated and realistic Lagrangians have been considered, some of them inspired directly by eq. 3.1. One such representative model, a direct predecessor of our considerations, was recently analyzed in [77]. Its Lagrangian, indexed by an auxiliary parameter m, has the form

$$L(x, \dot{x}) = (\dot{x} - 1)^{\frac{2m-1}{2m+1}} - V(x) \tag{3.2}$$

where the roots of this expression are always taken to be real, regardless of the actual sign of $\dot{x} - 1$. Since the corresponding momentum $p(x, \dot{x})$ is now a double-valued function, applying the usual Legendre transform on this Lagrangian results into a *pair* of Hamiltonians

$$H_{\pm} = p \pm \frac{1}{m-2}\, p^{\frac{1-2m}{2}} + V(x) \tag{3.3}$$

A curious result is obtained by choosing $m = 1$. In such case, the two branches of the *quantized* counterpart of eq. 3.3 are actually supersymmetric partners in the spirit of eq. 2.13, and might be written in the momentum space as $H_- = a^\dagger a$ and $H_+ = aa^\dagger$ with

$$(a\psi)(p) = \psi'(p) + \sqrt{p}\,\psi(p) \tag{3.4}$$

3.1.1 Our model

In [10], we have considered a Lagrangian, which may be seen as a direct generalization of eq. 3.2. The core of this generalization lies in the introduction of a general function $f(x)$ in place of the original $f(x) = -1$, making the resulting Lagrangian look as

$$L(x, \dot{x}) = C(\dot{x} + f(x))^{\frac{2m+1}{2m-1}} - \delta \qquad C = \left(\frac{1-2m}{1+2m}\right) \delta^{\frac{2}{1-2m}} \tag{3.5}$$

The normalization constant C is chosen with regard to future computations, with the auxiliary parameter δ being restricted to $\delta > 0$. In our considerations, we have omitted the explicit

presence of a potential function $V(x)$, which has to be discussed independently. The canonical momentum of our Lagrangian is given by

$$p(x,\dot{x}) = \frac{\partial L}{\partial \dot{x}} = -\delta^{\frac{2}{1-2m}}(\dot{x} + \gamma f(x))^{\frac{2}{2m-1}} \tag{3.6}$$

which can be easily inverted to yield the double-valued relation for the velocity $\dot{x}$, paralleling the result of [77]

$$\dot{x}(x,p) = -f(x) + \delta(\pm p)^{\frac{2m-1}{2}} \tag{3.7}$$

The corresponding Hamiltonian for a general m has consequently also a double-valued structure, expressed by its subscript

$$H_{\pm}(x,p) = -pf(x) - \frac{2\delta(\pm p)^{\frac{2m+1}{2}}}{2m+1} + \delta \tag{3.8}$$

The success of expressing this generalized double-valued Hamiltonian explicitly may be certainly encouraging, and provoke introduction of quantization schemes in parallel to [77]. Before we come to that, we discuss a special choice of $f(x)$, which shall link our general Lagrangian to a well-known evolution equation of great phenomenological interest.

The Lienard-type oscillator

One of the principal motivations for the introduction of eq. 3.5 has been the search for a classical as well as quantum dynamical description of a cubic oscillator being subject to a damped nonlinear force. Classically, this system may be described by an equation

$$\ddot{x} + kx\dot{x} + \frac{k^2}{9}x^3 + \lambda x = 0 \qquad \lambda > 0 \tag{3.9}$$

with $kx\dot{x}$ playing the role of the damping. This is a nonlinear autonomous differential equation of Liénard type. Such equations appear commonly in optics [80] as well as theory of Bose-Einstein condensates [81, 82]. However, the presence of the damping might be challenging, when one tries to quantize the system [83]. The Lagrangian description of the above system was examined in detail in [84], where a convenient Lagrange function leading to eq. 3.9 was found to be

$$L(x,\dot{x}) = \frac{27\lambda^3}{2k^2}\left(k\dot{x} + \frac{k^2x^2}{3} + 3\lambda\right)^{-1} + \frac{3\lambda\dot{x}}{2k} - \frac{9\lambda^2}{2k^2} \tag{3.10}$$

This Lagrangian, being convex in the velocities, does not provide any obstacles in transition to the corresponding Hamiltonian description, with the result

$$H(x,p) = \frac{9\lambda^2}{2k^2}\left(2 - 2\sqrt{1 - \frac{2kp}{3\lambda}} + \frac{k^2}{9\lambda} - \frac{2kp}{3\lambda} - \frac{2k^3x^2p}{27\lambda^2}\right) \tag{3.11}$$

Despite having such a nonstandard form, this Hamiltonian may be expressed as $H(x,p) = f(p)x^2 + U(p)$ for appropriately chosen functions $f(p)$ and $U(p)$. We shall see, that this Hamiltonian arises as a special case of eq. 3.8. As a first step, we set $m = 0$ in eq. 3.5, making the corresponding Hamiltonian degenerate into a deceptively simple form

$$H_{\pm}(x,p) = -pf(x) \mp 2\delta\sqrt{-p} + \delta \tag{3.12}$$

It is readily noticed that the real or the complex character of $H_{\pm}$ depends on the signs of the momentum p. In addition, once we specify the previously undetermined function $f(x)$ and the parameter δ to be

$$f(x) = \frac{\lambda}{2}x^2 + \frac{9\lambda^2}{2k^2}, \qquad \delta = \frac{9\lambda^2}{2k^2} \tag{3.13}$$

followed by a shift and translation $p \to \frac{2k}{3\lambda}p - 1$, we arrive at our desired Hamiltonian form of eq. 3.11 as a plus branch of the following double-valued expression

$$H_{\pm}(x,p) = \frac{9\lambda^2}{2k^2}\left[2 \mp 2\sqrt{1 - \frac{2kp}{3\lambda}} + \frac{k^2x^2}{9\lambda} - \frac{2kp}{3\lambda} - \frac{2k^3x^2p}{27\lambda^2}\right] \tag{3.14}$$

We have to stress that actually *both* of these Hamiltonians are equally plausible models for the nonlinear system of eq. 3.9. Furthermore, in both $H_{\pm}$, the presence of a linear harmonic oscillator potential is revealed in the limit $k \to 0$. Actually, as observed in [85], eq. 3.9 can always be converted to a harmonic oscillator form under the nonlocal transformation $U = xe^{\frac{k}{3}\int x(\tau)d\tau}$.

It is interesting to note, that the Lagrangian in eq. 3.10 is not the only one describing the damped cubic oscillator system. Already in [85], it was noted that an alternative, but still completely equivalent, description of dynamics is provided by the Lagrangian

$$L(x,\dot{x}) = \left(\frac{k^2x^2}{3} + 3\lambda - k\dot{x}\right)^{-1} \tag{3.15}$$

Using for the last time the machinery of Legendre transform leads first to the canonical momentum

$$p(x,\dot{x}) = \frac{\partial L}{\partial \dot{x}} = \frac{1}{k}\left(\frac{kx^2}{3} + \frac{3\lambda}{k} - \dot{x}\right)^{-2} \tag{3.16}$$

then, by inversion, to the (double-valued) expression for the velocity

$$\dot{x} = \frac{kx^2}{3} + \frac{3\lambda}{k} \pm \frac{1}{\sqrt{kp}} \tag{3.17}$$

and finally to an alternative double-valued Hamiltonian, which serves as a description of eq. 3.9, equivalent to eq. 3.8.

$$H_{\pm}(x,p) = \frac{k}{3}x^2p + \frac{3}{k}\lambda p \mp 2\sqrt{\frac{p}{k}} \tag{3.18}$$

The component H_+ for $k < 0$ has earlier been found to possess interesting $\lambda = 0$ limit [85]. Having two Hamiltonian description of the same system might appear superfluous, it shall however prove very handy in quantizing the system.

3.1.2 Quantization

Quantization of non-standard Hamiltonians $H(x,p) \neq p^2 + V(x)$ is a subject of active research, and must be definitely perceived more as a creative than algorithmic process. A particular scheme for quantizing Hamiltonians with variable mass

$$H(x,p) = \frac{p^2}{2m(x)} + V(x) \tag{3.19}$$

has been suggested by von Roos et al. in [86, 87]. The essence of their considerations is, that the quantized counterparts of eq. 3.19 can acquire a general form depending on three parameters α, β, γ

$$H = \frac{1}{4}\left(m^{\alpha}(x) i \frac{d}{dx} m^{\beta}(x) i \frac{d}{dx} m^{\gamma}(x)\right) + V(x) \tag{3.20}$$

as long as $\alpha + \beta + \gamma = -1$. Every quantum Hamiltonian satisfying this condition may be seen as a quantum counterpart of eq. 3.19, with the respective Hamiltonians being in general nonequivalent for different α, β, γ. This strategy was employed in [84] to quantize our Lienard-oscillator nonlinear system. The Hamiltonian of the system has precisely the form of eq. 3.19, only with p and x interchanged; $H(x,p) = x^2/2m(p) + V(p)$. The corresponding functions are

$$m(p) = \frac{1}{\lambda\left(1 - \frac{2k}{3\lambda}p\right)} \qquad U(p) = \frac{9\lambda^2}{2k^2}\left(\sqrt{1 - \frac{2k}{3\lambda}p} - 1\right)^2 \tag{3.21}$$

The quantized Hamiltonian is shown in [84] to possess remarkable results for parameters satisfying $4\alpha(\alpha + \beta + 1) = 1/4$. Under this condition, the corresponding Schrödinger equation becomes exactly solvable, with the spectrum becomes identical to the common linear harmonic oscillator.

In this note, we aim to extend the quantization scheme to our type-II Hamiltonian of eq. 3.18. Assuming $k > 0$, and by adapting the same procedure as outlined above, we end up with the Schrödinger equation

$$\frac{3}{kp} H_{\pm}(x,p) = -\frac{d^2}{dp^2} \mp \frac{6}{\sqrt{k^3 p}} + \frac{9}{k^2}\lambda \tag{3.22}$$

After the change of variables $p = r^2$ and $p\,\psi^{(\pm)}(p) = r^{3/2}\chi(r)$, we acquire the equation in a more natural-looking form

$$-\chi''(r) + \frac{3}{4r^2}\chi(r) + \frac{36}{k^2}r^2\chi(r) \mp \frac{24}{k^{3/2}}r\chi(r) = \frac{12}{k}E^{(\pm)}\chi(r) \tag{3.23}$$

This differential equation, to the best of our knowledge, cannot be solved exactly, due to the term linear in r. It is however well-suited for application of the Rayleigh-Schrödinger perturbation theory. As long as we denote $\mp\frac{24}{k^{3/2}}r = gV$, we may decompose the Hamiltonian together with its eigenvalues and eigenfunctions as

$$H = H_0 + gV, \qquad E = \sum_{m=0}^{\infty} g^m E_m \tag{3.24}$$

with H_0 denoting the radial harmonic oscillator Hamiltonian having eigenvalues $E_0^{(n)} = \omega(4n + 2l + 3)$ and frequency $\omega = 6s^{-1}$. In the next step, we would only have to insert these formulas into the Schrödinger equation and write down the corresponding eigenvalues

$$E_n^{(\pm)} = 2n + 2 \mp \xi_n \qquad n \in \mathbb{N}_0 \tag{3.25}$$

where ξ_n needs to be evaluated numerically. While the absence of solvability may seem daunting at first, it is actually a sign of a great progress. While the quantized form of eq. 3.11 essentially degenerates back to the common harmonic oscillator, applying the same procedure for eq. 3.18 yields a brand new quantum system, which provides a far more promising description for the quantum analogue of the damped cubic oscillator.

3.2 The inverse square root potential

Since a full classification of quantum potentials in the hypergeometric family has been achieved [49], the focus of researchers has turned to more general potentials, solvable in terms of Heun functions of various kinds. Recently, a potential with behavior closely related to the more famous hydrogen atom has been conjectured to contain interesting properties regarding its solvability [88]. The potential depends on the inverse square root of the radial coordinate, giving rise to the Schrödinger equation

$$-\psi''(x) - \frac{e^2}{\sqrt{x}}\psi(x) = E\psi(x) \tag{3.26}$$

acting on $(0, \infty)$ with $\psi(0) = 0$. In analogy with the hydrogen atom, the Hamiltonian may be expected to contain bands of bound-state and scattering energies. The fundamental idea of [88] is, that although eq. 3.26 itself gets solved in terms of tri-confluent Heun functions, the solution may be expressed using *derivatives* of much more accessible confluent hypergeometric functions

$$\psi(x) = e^{-kx}\frac{d}{dy}\left\{c_1 e^{-\sqrt{a}y}\,{}_1F_1\left(-\frac{a}{2}, \frac{1}{2}; y^2\right) + c_2 e^{-\sqrt{a}y} H_a(y)\right\}\Bigg|_{y=\sqrt{\delta x}+\sqrt{2a}} \tag{3.27}$$

with $k^2 = -E$ and $a = e^4/2k^3$. For future convenience, one of the solutions has been expressed using the Hermite function $H_a(x)$, which generalizes the notion of Hermite polynomials to arbitrary values of a, and which may be itself written in terms of hypergeometric functions

$$H_a(x) = 2^a\sqrt{\pi}\left\{\frac{1}{\Gamma(\frac{1-a}{2})}\,{}_1F_1\left(-\frac{a}{2}, \frac{1}{2}; z^2\right) - \frac{2z}{\Gamma(-\frac{a}{2})}\,{}_1F_1\left(-\frac{1-a}{2}, \frac{3}{2}; z^2\right)\right\} \tag{3.28}$$

In search for the eigenvalues, the general solution of eq. 3.26 must be complemented by conditions of normalizability, realized by the vanishing of the wavefunction at infinity. While this condition results in

$$\frac{c_1}{c_2} = \frac{2a\,{}_1F_1\left(1 - \frac{a}{2}, \frac{3}{2}, 2a\right) + {}_1F_1\left(-\frac{a}{2}, \frac{1}{2}; 2a\right)}{\sqrt{2a}H_{a-1}\left(\sqrt{2a}\right) - H_a\left(\sqrt{2a}\right)} \tag{3.29}$$

the boundary condition at the origin yields the final secular equation expressed in terms of Hermite functions, whose roots concide with the eigenvalues of eq. 3.26.

$$\sqrt{2a}H_{a-1}\left(-\sqrt{2a}\right) - H_a\left(-\sqrt{2a}\right) = 0 \tag{3.30}$$

Although this equation does not admit its roots to be expressed in a closed form, it allows in principle for solving to arbitrary precision, with the graphical result shown in fig. X. Furthermore, a high-precision approximation technique, outlined also in [88], enables us to express the n-th eigenvalue approximately as

$$E_n = -\left(\frac{e^2}{2}\right)^{4/3}\left(n - \frac{1}{2\pi}\right)^{-2/3} \tag{3.31}$$

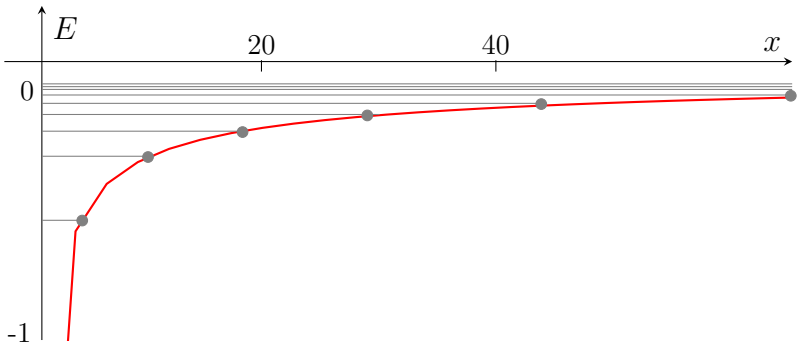

Figure X: *Bound states of the inverse square root potential well.*

3.2.1 Intermezzo: $\mathcal{PT}$-symmetrization of the hydrogen atom

We aim to define a consistent quasi-hermitian counterpart of the square-root potential by allowing general complex values of its coupling constant. With this in mind, it is instructive to review the procedure of $\mathcal{PT}$-symmetrizing the hydrogen atom [89, 90], a model whose role in the development of quantum theory can hardly be overemphasized. We shall express its Hamiltonian in its radial form, indexed by the angular momentum ℓ, and giving rise to a Schrödinger equation

$$-\psi''(x) + \frac{\ell(\ell+1)}{x^2}\psi(x) - \frac{e^2}{x}\psi(x) = E\psi(x) \qquad \ell = 0, 1, \ldots \tag{3.32}$$

defined again along the half-line $x \in (0, \infty)$. From physical viewpoint, the model contains a combination of the bound-state and scattering spectrum, demonstrating (historically for the first time), that confinement of electrons in atoms takes place only at sufficiently low energies. On the side of mathematics, the Hamiltonian has proven exactly solvable in terms of confluent hypergeometric functions. For the (negative) bound states with $E = -k^2$, one may express the general solution as$\psi(x) = c_1\psi_1(x) + c_2\psi_2(x)$ with

$$\begin{aligned}\psi_1(x) &= e^{-kx}x^{\ell+1}{}_1F_1\left(1+\ell-\frac{e^2}{2k}, 2\ell+2, 2kx\right)\\ \psi_2(x) &= e^{-kx}x^{-\ell}{}_1F_1\left(-\ell-\frac{e^2}{2k}, -2\ell, 2kx\right)\end{aligned} \tag{3.33}$$

Moreover, under standard physical boundary conditions, the confluent hypergeometric functions in eq. 3.33 degenerate to normalizable Laguerre polynomials, and the bound-state energy eigenvalues E_n become expressible in a closed form

$$E_n = -\frac{e^4}{2n^2} \tag{3.34}$$

These energies re-emerge also as poles of the scattering matrix, which may be curiously also expressed by a closed formula (together with the coefficients of transmission and reflection) as

$$S(k) = \frac{\Gamma\left(l+1+\frac{ie^2}{2k}\right)}{\Gamma\left(l+1-\frac{ie^2}{2k}\right)} \tag{3.35}$$

In [89] it has been shown, that most of the remarkable formal properties of this Hamiltonian survive also a modification provided by quasi-hermitian theory. The essence of this modification lies in replacing eq. 3.32 by a purely imaginary coupling term, the resulting equation being

$$-\psi''(x) + \frac{\ell(\ell+1)}{x^2}\psi(x) - \frac{ie^2}{x}\psi(x) = E\psi(x) \qquad \ell = 0, 1, \ldots \tag{3.36}$$

In order to remain in the domain of quantum mechanics and keep the spectrum of eq. 3.36 real, this change in the potential has to be complemented by a reinterpretation of the observable coordinate x. The new coordinate can be defined a number of ways, among which the authors of [89] have chosen the U-shaped complex curve $x(s)$ shown in fig. XI.

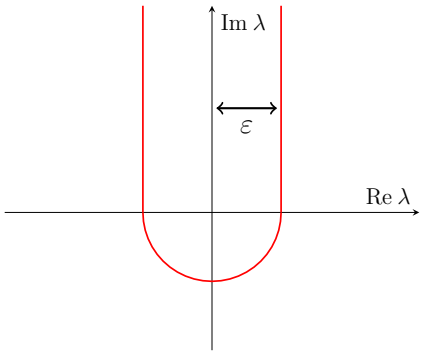

Figure XI: *A complex integration curve $x(s)$ of the $\mathcal{PT}$-symmetric Schrödinger eq. 3.36, which has been chosen instead of the usual real half-line $(0, \infty)$.*

In our definition, this curve admits a single degree of freedom, realized by the parameter ε and expressing the winding distance of the curve from the origin. The curve may be parametrized by a coordinate-like real variable $s \in (-\infty, \infty)$, with the result

$$x^U_{(\varepsilon)}(s) = \begin{cases} -i\left(s + \frac{\pi}{2}\varepsilon\right) - \varepsilon & s \in (-\infty, -\frac{\pi}{2}\varepsilon) \\ \varepsilon\, \exp\left\{i\left(\frac{s}{\varepsilon} + \frac{3\pi}{2}\right)\right\} & s \in (-\frac{\pi}{2}\varepsilon, \frac{\pi}{2}\varepsilon) \\ i\left(s - \frac{\pi}{2}\varepsilon\right) + \varepsilon & s \in (\frac{\pi}{2}\varepsilon, \infty) \end{cases} \tag{3.37}$$

This transition has a number of important consequences. First, the original integer-valued angular momentum ℓ loses this physical interpretation, and gets a new status of a mere real index parameter (which is no longer constrained to half-integer values).

Second, in order to stay in the realm of quantum mechanics, one has to impose a requirement of stability (boundedness from below) on the Hamiltonian. Without this condition, the Hamiltonian cannot play the role of energy of any measurable system. This has important consequences, since computing the spectrum of eq. 3.36 indeed demonstrates its instability [91]. A remedy proposed in [89] lies in the transition from a (positive) mass m to its negative counterpart $-m$, taking inspiration from a recent renewed interest in theories with indefinite or negative mass. In this setting, the bound states may be readily constructed as

$$E_{\pm n} = -\left(\frac{e^2}{2\ell + 1 \pm (2n+1)}\right)^2 \tag{3.38}$$

This spectrum is now safely bounded from below and moreover (curiously) independent on the parameter ε. In the subsequent considerations [90], it turned out that not only the eigenvalues, but also the scattering data of the newly emerged model can be obtained explicitly. We use the well-known $|z| \to \infty$ asymptotics of the hypergeometric function

$${}_1F_1(a, b, z) \sim \frac{\Gamma(b)}{\Gamma(b-a)} \frac{e^{i\pi a}}{z^a} + \frac{\Gamma(b)}{\Gamma(a)} e^z \tag{3.39}$$

valid for $0 < \arg z < \pi$ (where the term $e^{i\pi a}$ emerges when rotating the usual textbook result valid on $-\pi/2 < \arg z < \pi/2$). The infinite range of the Coulomb potential gets manifested in an additional term in the long-range asymptotics of the $\mathcal{PT}$-symmetrized model

$$\begin{aligned} \psi_j(s \to +\infty) &\sim a_{j+} \exp\left(iks + \frac{ie^2}{2k}\ln(2ks)\right) + b_{j+} \exp\left(-iks - \frac{ie^2}{2k}\ln(2ks)\right) \\ \psi_j(s \to -\infty) &\sim a_{j-} \exp\left(iks - \frac{ie^2}{2k}\ln(2ks)\right) + b_{j-} \exp\left(-iks + \frac{ie^2}{2k}\ln(2ks)\right) \end{aligned} \tag{3.40}$$

When computing the scattering quantities, one must take into account that the forward and backward coefficients of reflection and transmission are generally not equivalent for non-hermitian systems. Still, they may be expressed from eq. 3.40 in a sufficiently simple fashion in terms of a_j and b_j [92]. In the present case, the coefficients may be (after some formal manipulations) expressed in a very neat form

$$
\begin{aligned}
T_{L\to R}(k) &= \frac{a_{2+}b_{1+}-a_{1+}b_{2+}}{a_{2-}b_{1+}-a_{1-}b_{2+}} = \frac{i}{2\pi}e^{-i\pi k\varepsilon}\Gamma\left(-\ell-\frac{ie^2}{2k}\right)\Gamma\left(\ell+1-\frac{ie^2}{2k}\right)\\
R_{L\to R}(k) &= \frac{b_{1+}b_{2-}-b_{1-}b_{2+}}{a_{2-}b_{1+}-a_{1-}b_{2+}} = T_{L\to R}(k)\, e^{-2k\varepsilon}\,(\cos(2\pi\ell)-1)\\
T_{R\to L}(k) &= \frac{a_{2-}b_{1-}-a_{1-}b_{2-}}{a_{2-}b_{1+}-a_{1-}b_{2+}} = -T_{L\to R}(k)\\
R_{R\to L}(k) &= \frac{a_{1+}a_{2-}-a_{1-}a_{2+}}{a_{2-}b_{1+}-a_{1-}b_{2+}} = T_{R\to L}(k)\, e^{2k\varepsilon}
\end{aligned}
\tag{3.41}
$$

which readily reproduces the bound-states from eq. 3.38 as poles of $T_{R\to L}$. The natural step in this moment would lie in using the tools of quasi-hermitian theory to construct certain admissible set of physical metrics Θ for this $\mathcal{PT}$-symmetrized Hamiltonian. This is however conjectured to be a difficult task, and numerous attempts for such construction have been proven unsuccessful over the years.

3.2.2 Asymptotic analysis and scattering

Here we aim to generalize the considerations of the previous section to the inverse square root potential. We shall not consider the bound-state regime, and focus instead solely on the scattering scenario. This most certainly motivates further research, as bound states certainly exist for the $\mathcal{PT}$-symmetrized inverse square root model, and it is customary to know whether they correspond to real eigenvalues.

Regarding the asymptotics, we might once again make advantage of eq. 3.27. Although the asymptotic theory of general Heun functions is currently not very well explored, using this relationship brings the problem down to determining the asymptotics of confluent hypergeometric functions, a problem discussed already in eq. 3.39. On the real line, the long-range asymptotics may be computed by simple insertion as

$$
\psi(x) \sim \exp\left(ikx - \frac{e^2}{k}\sqrt{ix} - \frac{e^4}{8k^3}\ln(ix)\right) \qquad \text{for } x\to\infty \tag{3.42}
$$

The situation gets slightly counterintuitive when we move to the complex asymptotic domain of x and to a non-hermitian, $\mathcal{PT}$-symmetric version of the Hamiltonian defined on the exactly same contour as the hydrogen atom, depicted in fig. XI. The choice of the contour is again guided by a close similarity of the inverse square root and Coulomb hamiltonians (different choices of the contour are successful for infinite potential wells, see [93]). In this scenario, we obtain a *pair* of independent asymptotic solutions of our $\mathcal{PT}$-symmetric Schrödinger equation (parametrized again by $x[s]$) as

$$
\begin{aligned}
\psi_j(x) &\sim a_{j-}\exp\left(-\frac{i\delta s}{2}+\sqrt{2a\delta \mathrm{i}s}+a\ln(\mathrm{i}s)\right)+b_{j-}\exp\left(\frac{i\delta s}{2}-\sqrt{2a\delta \mathrm{i}s}-a\ln(\mathrm{i}s)\right)\\
\psi_j(x) &\sim a_{j+}\exp\left(-\frac{i\delta s}{2}+\sqrt{2a\delta \mathrm{i}s}+a\ln(\mathrm{i}s)\right)+b_{j+}\exp\left(\frac{i\delta s}{2}-\sqrt{2a\delta \mathrm{i}s}-a\ln(\mathrm{i}s)\right)
\end{aligned}
\tag{3.43}
$$

which indeed degenerate to the usual plane waves whenever $e \to 0$, or equivalently $a \to 0$. These plane-like waves are again deformed by two non-negligible subdominant contributions, induced by the infinite range of the potential. Nevertheless, we may still treat them as incoming and outcoming waves and use the powerful machinery of scattering theory. Making the analogy with the hydrogen atom complete, we compute the respective coefficients

$$\begin{aligned}
a_{1+} &= c_1\, e^{\mathrm{i}\delta\pi\varepsilon/4} e^{-\delta\varepsilon/2} e^{-2a} \frac{\sqrt{2a}}{\Gamma\left(\frac{1+a}{2}\right)} \qquad & b_{1+} &= c_1\, e^{-\mathrm{i}\delta\pi\varepsilon/4} e^{\delta\varepsilon/2} e^{2a} \frac{a}{\Gamma\left(\frac{2-a}{2}\right)} \\
a_{1-} &= c_1\, e^{-\mathrm{i}\delta\pi\varepsilon/4} e^{-\delta\varepsilon/2} e^{2a} \frac{a}{\Gamma\left(\frac{2-a}{2}\right)} \qquad & b_{1-} &= c_1\, e^{\mathrm{i}\delta\pi\varepsilon/4} e^{\delta\varepsilon/2} e^{-2a} \frac{\sqrt{2a}}{\Gamma\left(\frac{1+a}{2}\right)} \\
a_{2+} &= c_2\, e^{\mathrm{i}\delta\pi\varepsilon/4} e^{-\delta\varepsilon/2} e^{-2a} \frac{-\sqrt{2a}}{\Gamma\left(\frac{2+a}{2}\right)} \qquad & b_{2+} &= c_2\, e^{-\mathrm{i}\delta\pi\varepsilon/4} e^{\delta\varepsilon/2} e^{2a} \frac{1-a}{\Gamma\left(\frac{3-a}{2}\right)} \\
a_{2-} &= c_2\, e^{-\mathrm{i}\delta\pi\varepsilon/4} e^{-\delta\varepsilon/2} e^{2a} \frac{1-a}{\Gamma\left(\frac{3-a}{2}\right)} \qquad & b_{2-} &= c_2\, e^{\mathrm{i}\delta\pi\varepsilon/4} e^{\delta\varepsilon/2} e^{-2a} \frac{-\sqrt{2a}}{\Gamma\left(\frac{2+a}{2}\right)}
\end{aligned} \tag{3.44}$$

from which the final coefficients of transmission and reflection may be computed. In this case, the factorization process simplifying the results does not occur, so that we are left with the more complicated formulas

$$\begin{aligned}
T_{L\to R} &= \frac{a_{2+}b_{1+} - a_{1+}b_{2+}}{a_{2-}b_{1+} - a_{1-}b_{2+}} = e^{i\delta\pi\varepsilon/2} e^{-4a} \frac{\frac{-\sqrt{2a^3}}{\Gamma(\frac{2+a}{2})\Gamma(\frac{2-a}{2})} - \frac{\sqrt{2a(1-a)}}{\Gamma(\frac{1+a}{2})\Gamma(\frac{3-a}{2})}}{\frac{\sqrt{2a}(1-a)}{\Gamma(\frac{2-a}{2})\Gamma(\frac{3-a}{2})} - \frac{a(1-a)}{\Gamma(\frac{2+a}{2})\Gamma(\frac{3-a}{2})}} \\
R_{L\to R} &= \frac{b_{1+}b_{2-} - b_{1-}b_{2+}}{a_{2-}b_{1+} - a_{1-}b_{2+}} = e^{i\delta\pi\varepsilon/2} e^{-4a} \frac{\frac{-\sqrt{2a}(1-a)}{\Gamma(\frac{2+a}{2})\Gamma(\frac{3-a}{2})} - \frac{\sqrt{2a^3}}{\Gamma(\frac{1+a}{2})\Gamma(\frac{2-a}{2})}}{\frac{a(1-a)}{\Gamma(\frac{2-a}{2})\Gamma(\frac{3-a}{2})} - \frac{a(1-a)}{\Gamma(\frac{2-a}{2})\Gamma(\frac{3-a}{2})}} \\
T_{R\to L} &= \frac{a_{2-}b_{1-} - a_{1-}b_{2-}}{a_{2-}b_{1+} - a_{1-}b_{2+}} = e^{i\delta\pi\varepsilon/2} e^{-4a} \frac{\frac{-\sqrt{2a^3}}{\Gamma(\frac{3+}{2})\Gamma(\frac{1+a}{2})} - \frac{\sqrt{2a(1-a)}}{\Gamma(\frac{2+a}{2})\Gamma(\frac{3-a}{2})}}{\frac{a(1-a)}{\Gamma(\frac{2-a}{2})\Gamma(\frac{2-a}{2})} - \frac{a(1+a)}{\Gamma(\frac{2-a}{2})\Gamma(\frac{3-a}{2})}} \\
R_{R\to L} &= \frac{a_{1+}a_{2-} - a_{1-}a_{2+}}{a_{2-}b_{1+} - a_{1-}b_{2+}} = e^{i\delta\pi\varepsilon/2} e^{-4a} \frac{\frac{-\sqrt{2a}(1-a)}{\Gamma(\frac{1+a}{2})\Gamma(\frac{2-a}{2})} - \frac{\sqrt{2a^3}}{\Gamma(\frac{2+a}{2})\Gamma(\frac{3-a}{2})}}{\frac{a(1-a)}{\Gamma(\frac{2-a}{2})\Gamma(\frac{3-a}{2})} - \frac{a(1-a)}{\Gamma(\frac{2-a}{2})\Gamma(\frac{3-a}{2})}}
\end{aligned} \tag{3.45}$$

Such behavior is completely expected, since the factorization of transmission coefficients would lead to (nonexistent) closed-form expressions for the spectrum. A recent idea, which could in principle solve this apparently troubling phenomenon [94], suggests that solvability may be reestablished by generalizing the inverse square root potential into

$$V(x) = \frac{\alpha_1}{\sqrt{x}} + \frac{\alpha_2}{x} + \frac{\alpha^3}{x^{3/2}} \tag{3.46}$$

and making a certain convenient choice of the parameters α_i. This phenomenon is usually referred to as conditionally exact solvability in the literature [95].

Chapter 4

Applications to realistic finite-dimensional models

In the usual quantum description of bosonic systems, the underlying Hilbert space is always assumed infinite-dimensional. This is a necessary consequence of the Stone-Von Neumann theorem about unitary representations of canonical commutation relations ([14], thm. 8.2.4). On the other hand, fermionic anticommutation relations can be (and most often are) unitarily represented in a finite-dimensional Hilbert space. Fermionic systems are of course ubiquitous in quantum mechanics, and form the very core for the theories of condensed matter and solid state. This alone provides a strong motivation for studying finite-dimensional quasi-hermitian operators [96, 97].

Finite-dimensional Hamiltonians may be also regarded as approximate description of bosonic systems. Because of their mathematical simplicity, they can be used to address phenomena difficult to describe in infinite dimensions. Quasi-hermitian operators are no exception to this rule. They have been used to model quantum phase transitions [9], quantum catastrophes [8] or simplified big-bang scenarios [98]. The objects of interest in these models are the exceptional points [64, 99], which emerge inevitably on boundaries of observability domains.

4.1 The Su-Schrieffer-Heeger model

The Su-Schrieffer-Heeger (SSH) model is a simple many-body system, originally introduced in [100] to describe a 1D array of polyacetylene, shown in fig. XII. Thanks to its nontrivial spectral properties, it has later found numerous applications in solid state theory, most recently as a simple conceptual example of a topological insulator [101].

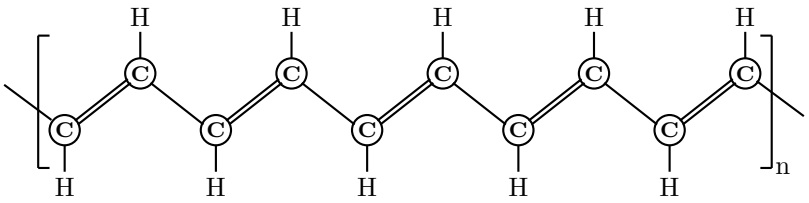

Figure XII: *Chain of polyacetylene, which motivated introduction of the SSH model*

The difference between the single and the double bonds in the above scheme is governed by the control parameter called θ, which shall be allowed to vary continuously. The number of polymerized sites is denoted by $n \in \mathbb{N}$. so that the number of carbon atoms is $2n$. We write the SSH Hamiltonian in its second-quantized form

$$H_{SSH}^{(n)} = \sum_{i=1}^{n} \left\{ t(1 - \Delta \cos\theta) a_{2i-1}^{\dagger} a_{2i} + t(1 + \Delta \cos\theta) a_{2i}^{\dagger} a_{2i+1} + h.c. \right\} \tag{4.1}$$

with $h.c.$ denoting hermitian conjugate, and $a_i^{\dagger}$, a_i being i-th site fermionic creation and annihilation operators. We can safely assume that $t = \Delta = 1$, since the physical properties of the system are not altered by those parameters. Furthermore, we also rescale the control parameter as $\lambda = \cos\theta$. The SSH model has two topologically distinct phases depending on the value of λ, as may be seen in fig. XIII. For $\lambda > 0$, there is an extra state (usually called the edge state), which completely changes its spectral topology.

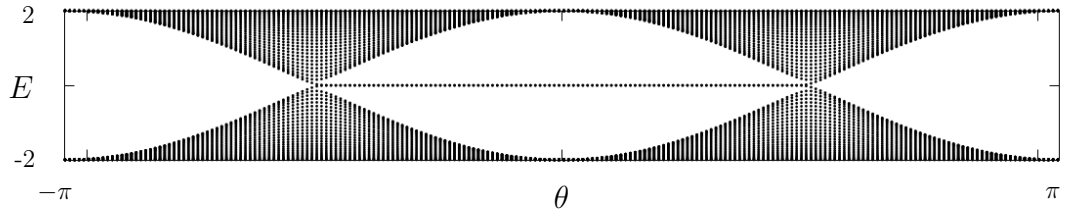

Figure XIII: *Spectrum of the $n = 50$ hermitian SSH model as a function of θ, demonstrating two topologically distinct phases.*

Since we are dealing with a non-interacting system, it is possible to substitute the usual $2^{2n} \times 2^{2n}$ Fock matrix representation by a $2n \times 2n$ matrix, whose (ij)-th element is the coefficient in front of $a_i^{\dagger} a_j$. This matrix shares the spectrum (though not the degeneracies) with the actual SSH model (see [102], thm. 7.1.1), and the spectrum spectrum may be expressed exactly as $E(k) = \pm\sqrt{2 + 2\cos^2\theta + 2(1 - \cos^2\theta)\cos k}$. In a recent paper [103], the authors suggested to complement the hermitian SSH model with a non-hermitian interaction term

$$H_I = i\gamma a_1^{\dagger} a_1 - i\gamma a_n^{\dagger} a_n \tag{4.2}$$

which may be understood as a complemented source and sink of equal strength. The resulting Hamiltonian $H = H_{SSH} + H_I$ is not hermitian, it is however manifestly $\mathcal{PT}$-symmetric. Its spectrum can be no longer expressed through a closed formula, but numerical experiments indicate, that its eigenvalues remain real for γ sufficiently small. Using the $2n \times 2n$ non-interacting representation, the matrix Hamiltonian can be written (for $n = 2$, with higher dimensions analogically) as

$$H^{(2)} = \begin{bmatrix} \gamma & -1-\lambda & & \\ -1-\lambda & & -1+\lambda & \\ & -1+\lambda & & -1-\lambda \\ & & -1-\lambda & \gamma^* \end{bmatrix} \tag{4.3}$$

Note that in [103], the authors only examined the case of γ being purely imaginary. The effects of general complex γ are illustrated in fig. XIV for three particular values of $\gamma = \rho + i\omega$. As a general feature, the bulk states are largely unaffected by modification of the parameters. On the other hand, the edge state behaves very sensitively to such perturbations and might even completely change the resulting topology.

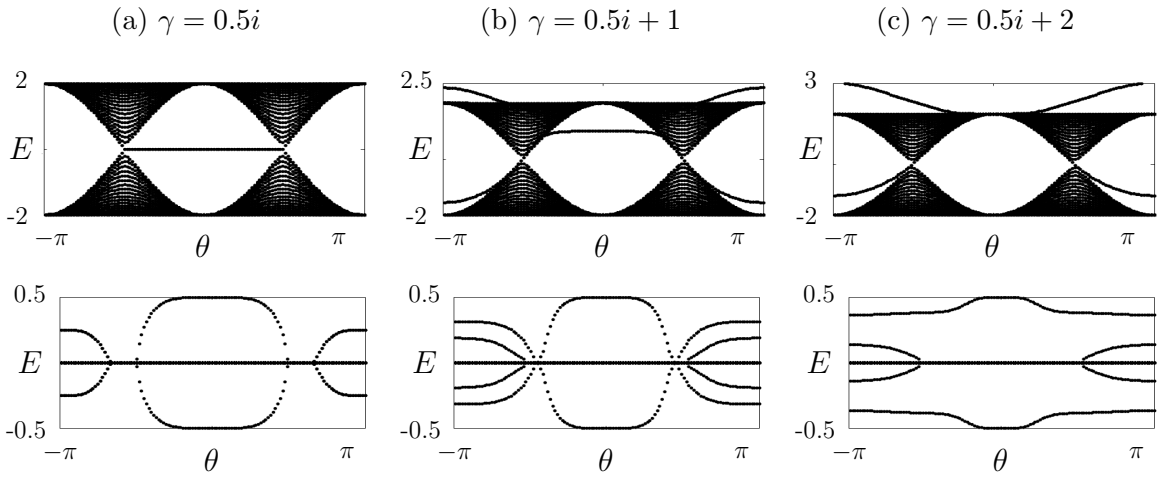

Figure XIV: *Real and complex parts of the spectrum for* $H_{SSH} + H_I$ *with* $n = 100$.

In the forthcoming search for metrics for our non-hermitian model, we shall start with discussing the special case $\lambda = 0$ separately. Curiously enough, such Hamiltonian was discovered independently by applying equidistant discretization methods to a $\mathcal{PT}$-symmetric Laplacian on a finite real interval, say $[-1, 1]$, subject to complex Robin boundary conditions

$$\psi'(\pm 1) = (\pm i\alpha + \beta)\psi(\pm 1) \tag{4.4}$$

with $\alpha, \beta \in \mathbb{R}$. This is one of the few infinite-dimensional quasi-hermitian Hamiltonians known to admit a metric to be constructed explicitly, at least for $\beta = 0$ [104, 105]. In the subsequent examination of its discretized counterpart, a complete analogy of this metric was constructed also for any finite dimension [106],. The relationship between the $\lambda = 0$ SSH model and the discretized Laplacian may be expressed through a nonlinear coordinate transformation

$$\omega = \frac{\beta}{(1-\alpha)^2 + \beta^2} \qquad \rho = \frac{1-\alpha}{(1-\alpha)^2 + \beta^2} \tag{4.5}$$

The domains of quasi-hermicity in the parameter space using both coordinate systems are shown in fig. XV. Their non-shrinking behavior of these domains in the limit $n \to \infty$ is just another manifestation of the nontrivial infinite-dimensional limit operator of eq. 4.4.

4.1.1 The universal metric

Finite-dimensional operators are by definition open to construction of the general metric numerically, in principle to arbitrary precision. However, our aim in this section is to obtain the results exactly in terms of closed formulas. Before we proceed further, we make precise the

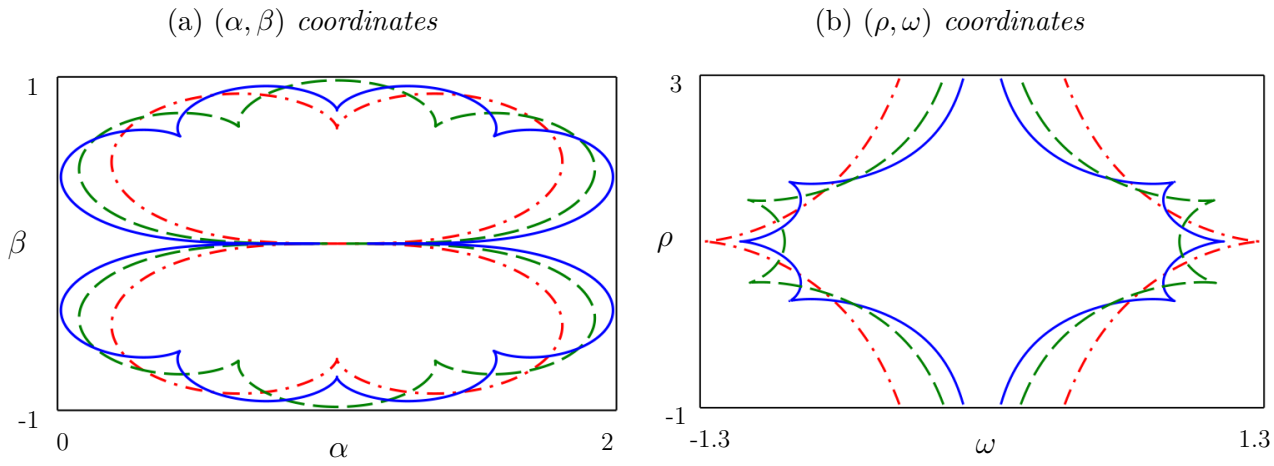

Figure XV: *Boundaries of observability domains for the* $\lambda = 0$ *SSH model, drawn for* $n = 3$ *(blue)* $n = 4$ *(green) and* $n = 5$ *(red).*

concept of universal metric for finite-dimensional operators. On a Hilbert space of dimension n and for a given quasi-hermitian operator H, the most general metric operator has n degrees of freedom and can be written as

$$\Theta = \sum_{k=1}^{n} \kappa_n |n\rangle\langle n| \tag{4.6}$$

where $|n\rangle$ are the eigenvectors of $H^\dagger$ and $\kappa_n > 0$. This $n \times n$ metric with n degrees of freedom is then called the universal metric. In principle, we could always compute these eigenvectors and express Θ through the formula above. This is however not very effective in general, as the actual possibility of computing such eigenvectors diminishes quickly with growing n. We use another method, much more useful in practice. For sufficiently small dimensions, we manipulate the equation symbolically (using any computed algebra program) and try to isolate patterns valid also for higher dimensions.

In order to use such strategy, we have to drop the condition of positivity for eq. 4.6. The resulting object is usually called a pseudometric and denoted by the letter $\mathcal{P}$. Again, this general pseudometric has n degrees of freedom, and thus can be expressed as a linear combination of n matrices. The search for such matrices shall occupy a central portion of the following text. As for eq. 4.3 with $\lambda = 0$, we arrive at the $n = 4$ result

$$\mathcal{P}^{(1)} = \begin{bmatrix} 1 & -\mathrm{i}\omega & -\mathrm{i}\omega\xi & -\mathrm{i}\omega\xi^2 \\ \mathrm{i}\omega & 1 & -\mathrm{i}\omega & -\mathrm{i}\omega\xi \\ \mathrm{i}\omega\xi^* & \mathrm{i}\omega & 1 & -\mathrm{i}\omega \\ \mathrm{i}\omega\xi^{*2} & \mathrm{i}\omega\xi^* & \mathrm{i}\omega & 1 \end{bmatrix} \quad \mathcal{P}^{(2)} = \begin{bmatrix} & 1 & -\mathrm{i}\omega & -\mathrm{i}\omega\xi \\ 1 & \rho & 1 & -\mathrm{i}\omega \\ \mathrm{i}\omega & 1 & \rho & 1 \\ \mathrm{i}\omega\xi^* & \mathrm{i}\omega & 1 & \end{bmatrix}$$

$$\mathcal{P}^{(3)} = \begin{bmatrix} & 1 & -\mathrm{i}\omega \\ 1 & \rho & 1 \\ 1 & \rho & 1 \\ \mathrm{i}\omega & 1 & \end{bmatrix} \quad \mathcal{P}^{(4)} = \begin{bmatrix} & & 1 \\ & 1 & \\ 1 & & \\ 1 & & \end{bmatrix} \tag{4.7}$$

where we denoted $\xi = \rho - \mathrm{i}\omega$. Note that $\mathcal{P}^{(1)}$ is positive by itself and generalizes the $\rho = 0$ result of [106], while $\mathcal{P}^{(4)}$ realizes a discrete operator of parity (and shows that the model is $\mathcal{PT}$-symmetric in the usual sense). This result clearly suggests an extrapolation pattern for higher n. In this pattern, the pseudometric with subscript k has $2(n-k)+1$ nonzero antidiagonals, with the nonzero elements listed in tab. A.

element	position
$-\mathrm{i}\omega\xi^{i-j-k}$	$i-j \geq k$
$\mathrm{i}\omega\xi^{*(i-j-k)}$	$j-i \geq k$
ρ	$\lvert i-j\rvert < k,\ i+j-k$ even
1	$\lvert i-j\rvert < k,\ i+j-k$ odd

Table A: *Nonzero elements of the pseudometric* $\mathcal{P}^{(k)}_{ij}$ *for the SSH model of eq. 4.1 with* $\lambda = 0$.

This scheme was successfully verified up to $n = 12$ in subsequent computations. Alternatively, one could prove the general result by double induction on n and k, following the footsteps of *prop. 2* in [106]. This result is certainly encouraging, since having a complete set of pseudometrics obtainable in a closed form is a rare property even among finite-dimensional Hamiltonians.

Having successfully constructed a complete set of pseudometrics, the final part of our task would, in principle, consist of verifying the condition of positivity of the resulting general n-parametric linear combination of $\mathcal{P}^{(k)}$. This is greatly simplified by the fact, that the pseudometric $\mathcal{P}^{(1)}$ is positive by itself, and thus a genuine metric. Consequently, we might employ the powerful machinery of perturbation theory and write

$$\Theta = \mathcal{P}^{(1)} + \varepsilon_2 \mathcal{P}^{(2)} + \cdots + \varepsilon_n \mathcal{P}^{(n)} \tag{4.8}$$

where the range of ε_i preserving the positivity of Θ has to be in general determined numerically. For purposes of clarity, we address shortly another special case, $\gamma = 0$ with λ arbitrary. Such model is manifestly hermitian, which however does not stop the quasi-hermitian machinery from working. As long as we denote $+ = 1+\lambda$ and $- = 1-\lambda$, we may write

$$\mathcal{P}^{(1)} = \begin{bmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & & 1 \end{bmatrix} \quad \mathcal{P}^{(2)} = \begin{bmatrix} & - & & \\ + & & + & \\ & - & & - \\ & & + & \end{bmatrix} \quad \mathcal{P}^{(3)} = \begin{bmatrix} & & 1 & \\ & 1 & & 1 \\ 1 & & 1 & \\ & 1 & & \end{bmatrix} \quad \mathcal{P}^{(4)} = \begin{bmatrix} & & & - \\ & & + & \\ & - & & \\ + & & & \end{bmatrix} \tag{4.9}$$

The formulas for general $n \in \mathbb{N}$ are clear from these expressions, with the nonzero elements (arranged again into a chessboard pattern) acquiring just three possible values $1, +, -$. Finally, we aim to merge together the results for nonzero λ and γ. In order to do this, we formulate a general ansatz, taking inspiration from results for both $\gamma = 0$ and $\lambda = 0$, and summarized for $n = 6$ in fig. XVI.

Inserting this ansatz into eq. 1.2 with our non-hermitian SSH Hamiltonian should in principle give us the values of the *a priori* unknown constants c_{ij} and the (real) terms corresponding to the green dots. Alas, numerical experiments indicate the emergence of a cutoff term breaking

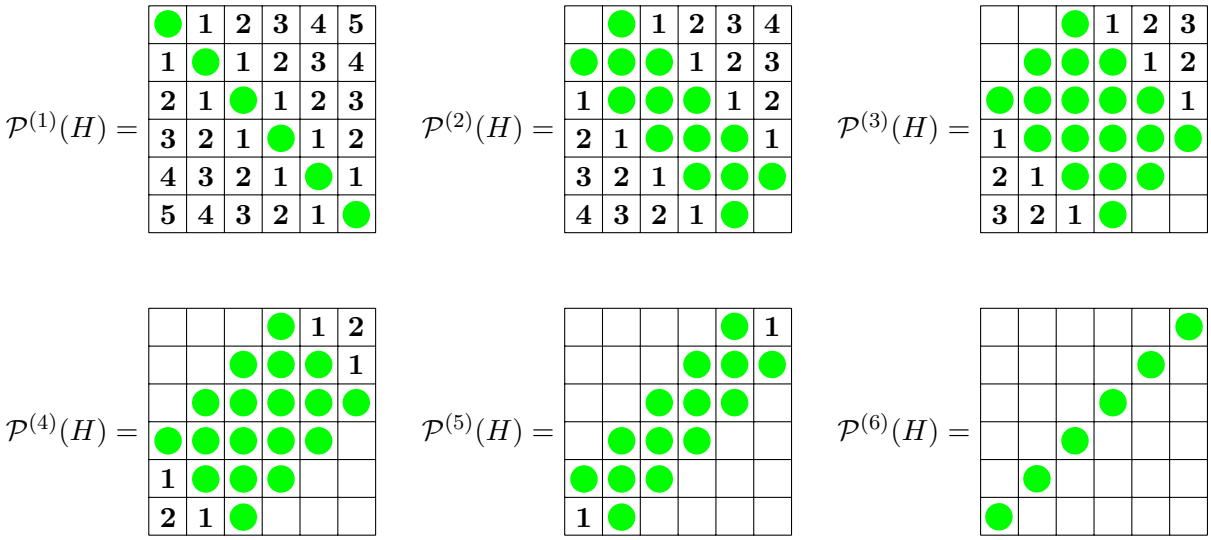

Figure XVI: *Ansatz for the pseudometrics for eq. 4.11 and $n = 6$. Green dots are real entries, $n \in \mathbb{N}$ stands for $c\, i^n \omega(\omega - i\rho)^{n-1}$ with c to be determined.*

the ansatz already for $n = 6$. As an example, consider the metric $\Theta = \mathcal{P}^{(1)}$, which could be inserted into fig. XVI to become

$$\Theta = \begin{bmatrix} 1 & -\frac{i\omega}{1+\lambda} & -\frac{\omega(\omega-i\rho)}{1-\lambda^2} & \frac{i\omega(\omega-i\rho)^2}{(1-\lambda^2)(1+\lambda)} & \frac{\omega(\omega-i\rho)^3}{(1-\lambda^2)^2} & \Lambda \\ \frac{i\omega}{1+\lambda} & 1 & -\frac{i\omega}{1-\lambda} & -\frac{\omega(\omega-i\rho)}{1-\lambda^2} & \frac{i\omega(\omega-i\rho)^2}{(1-\lambda^2)(1-\lambda)} & \frac{\omega(\omega-i\rho)^3}{(1-\lambda^2)^2} \\ -\frac{\omega(\omega+i\rho)}{1-\lambda^2} & \frac{i\omega}{1-\lambda} & 1 & -\frac{i\omega}{1+\lambda} & -\frac{\omega(\omega-i\rho)}{1-\lambda^2} & \frac{i\omega(\omega-i\rho)^2}{(1-\lambda^2)(1+\lambda)} \\ \frac{-i\omega(\omega+i\rho)^2}{(1-\lambda^2)(1+\lambda)} & -\frac{\omega(\omega+i\rho)}{1-\lambda^2} & \frac{i\omega}{1+\lambda} & 1 & -\frac{i\omega}{1-\lambda} & -\frac{\omega(\omega-i\rho)}{1-\lambda^2} \\ \frac{\omega(\omega+i\rho)^3}{(1-\lambda^2)^2} & \frac{-i\omega(\omega+i\rho)^2}{(1-\lambda^2)(1-\lambda)} & -\frac{\omega(\omega+i\rho)}{1-\lambda^2} & \frac{i\omega}{1-\lambda} & 1 & -\frac{i\omega}{1+\lambda} \\ \Lambda^* & \frac{\omega(\omega+i\rho)^3}{(1-\lambda^2)^2} & \frac{-i\omega(\omega+i\rho)^2}{(1-\lambda^2)(1+\lambda)} & -\frac{\omega(\omega+i\rho)}{1-\lambda^2} & \frac{i\omega}{1+\lambda} & 1 \end{bmatrix} \tag{4.10}$$

The outermost terms are, however, incompatible with the remaining condition of quasi-hermicity, and our natural-looking ansatz does not produce the desired results. This makes the analysis of our model difficult in higher dimensions, and most likely crushes the hopes for constructing a closed-form metric in its infinite-dimensional limit. While this is certainly an unpleasant feature, it can be very curiously remedied with just a slight modification of the original Hamiltonian. The modification, which draws its inspiration from [107], has the form

$$H^{(4)} = \begin{bmatrix} \rho + i\omega & -1-\lambda & & \\ -1+\lambda & & -1+\lambda & \\ & -1-\lambda & & -1-\lambda \\ & & -1+\lambda & \rho - i\omega \end{bmatrix} \tag{4.11}$$

For brevity, we shall refer to this modified Hamiltonian as the *dual SSH* model. The procedure of constructing its pseudometrics is completely parallel to eq. 4.3. For $\gamma = 0$, the chessboard pattern of eq. 4.9 may be reproduced in a slightly altered form, with the the odd pseudometrics now having entries varying with λ, and even pseudometrics having entries constant throughout the matrix. For $\pm = (1 \pm \lambda)$, this reads

$$\mathcal{P}^{(1)} = \begin{bmatrix} + & & & \\ & - & & \\ & & + & \\ & & & - \end{bmatrix} \quad \mathcal{P}^{(2)} = \begin{bmatrix} & 1 & & \\ 1 & & 1 & \\ & 1 & & 1 \\ & & 1 & \end{bmatrix} \quad \mathcal{P}^{(3)} = \begin{bmatrix} & & + & \\ & - & & - \\ + & & + & \\ & - & & \end{bmatrix} \quad \mathcal{P}^{(4)} = \begin{bmatrix} & & & 1 \\ & & 1 & \\ & 1 & & \\ 1 & & & \end{bmatrix} \tag{4.12}$$

This pattern is again very simple and admits expressing the results comfortably for any $n \in \mathbb{N}$. In order to provide direct comparison with SSH model for $\gamma = 0$, we list the nonzero matrix entries for both kinds of pseudometrics in tab. B.

	SSH		**dual SSH**
$+$	k even, $i-j$ odd	$+$	k odd, $i-j$ odd
$-$	k even, $i-j$ even	$-$	k odd, $i-j$ even
1	k odd	1	k even

Table B: Values of $\mathcal{P}^{(k)}_{ij}$ for eq. 4.1 and eq. 4.11.

The main result of the present section comes by applying the ansatz of eq. 4.10 on this operator. Discouraged by the negative results for eq. 4.3, it is curious enough that for the dual SSH model, the ansatz actually works flawlessly and provides a complete description of the physical Hilbert spaces for the Hamiltonian under consideration (again, a direct proof of this assertion could be in principle very complicated, but the evidence provided by symbolic manipulations is overwhelming).

Moreover, the undetermined coefficients in the ansatz acquire surprisingly simple forms (whose precise pattern, however, remains yet to isolate). Since the formulas are in general still too complicated to be printed explicitly, we content ourselves with showing the equivalent of eq. 4.10, which becomes

$$\Theta = \begin{bmatrix} 1+\lambda & -i\omega & -\frac{\omega(\omega-i\rho)}{1-\lambda} & \frac{i\omega(\omega-i\rho)^2}{1-\lambda^2} & \frac{\omega(\omega-i\rho)^3}{(1-\lambda)(1-\lambda^2)} & \frac{-i\omega(\omega-i\rho)^4}{(1-\lambda^2)^2} \\ i\omega & 1-\lambda & -i\omega & -\frac{\omega(\omega-i\rho)}{1+\lambda} & \frac{i\omega(\omega-i\rho)^2}{1-\lambda^2} & \frac{\omega(\omega-i\rho)^3}{(1+\lambda)(1-\lambda^2)} \\ -\frac{\omega(\omega+i\rho)}{1-\lambda} & i\omega & 1+\lambda & -i\omega & -\frac{\omega(\omega-i\rho)}{1-\lambda} & \frac{i\omega(\omega-i\rho)^2}{1-\lambda^2} \\ \frac{-i\omega(\omega+i\rho)^2}{1-\lambda^2} & -\frac{\omega(\omega+i\rho)}{1+\lambda} & i\omega & 1-\lambda & -i\omega & -\frac{\omega(\omega-i\rho)}{1+\lambda} \\ \frac{\omega(\omega+i\rho)^3}{(1-\lambda)(1-\lambda^2)} & \frac{-i\omega(\omega+i\rho)^2}{1-\lambda^2} & -\frac{\omega(\omega+i\rho)}{1-\lambda} & i\omega & 1+\lambda & -i\omega \\ \frac{i\omega(\omega+i\rho)^4}{(1-\lambda^2)^2} & \frac{\omega(\omega+i\rho)^3}{(1+\lambda)(1-\lambda^2)} & \frac{-i\omega(\omega+i\rho)^2}{1-\lambda^2} & -\frac{\omega(\omega+i\rho)}{1+\lambda} & i\omega & 1-\lambda \end{bmatrix} \tag{4.13}$$

4.2 Imaginary local interactions

Zero-range interaction Hamiltonians are with no doubt the best understood class of quantum operators, be it differential or discrete ones. While their differential realizations coincide with the class of Schrödinger operators, their discrete counterparts are studied less systematically, despite having well understood spectral properties [108, 53]. It comes as no surprise, that these operators have already received substantial attention also in the context of finite-dimensional quasi-hermitian theory [109, 110, 111].

In the previous section, we examined the non-hermitian SSH Hamiltonian, and found the results exceptionally accessible for $\lambda = 0$. This motivates a more general discussion with the interaction terms no longer constrained to the boundaries of the system. We start with a completely general Hamiltonian subject to imaginary zero-range interaction, the only constraint being the condition of $\mathcal{PT}$-symmetry (for simplicity, we also restrict attention to even space dimensions). The resulting $2n$-dimensional operator depends on n free parameters as

$$H^{(2n)} = \begin{bmatrix} i\alpha & -1 & & & \\ -1 & i\beta & -1 & & \\ & \ddots & & & \\ & & -1 & -i\beta & -1 \\ & & & -1 & -i\alpha \end{bmatrix} \tag{4.14}$$

with the parameters being denoted by Greek letters in alphabetical order. Although the quickly rising number of parameters makes the model very complicated with growing dimension, the reward may be seen in the vast diversity of its spectral properties. This is demonstrated even in the next-to-trivial case $n = 6$. The graphical results are shown in fig. XV, where one of the parameters is always set to zero in order to allow two-dimensional plotting.

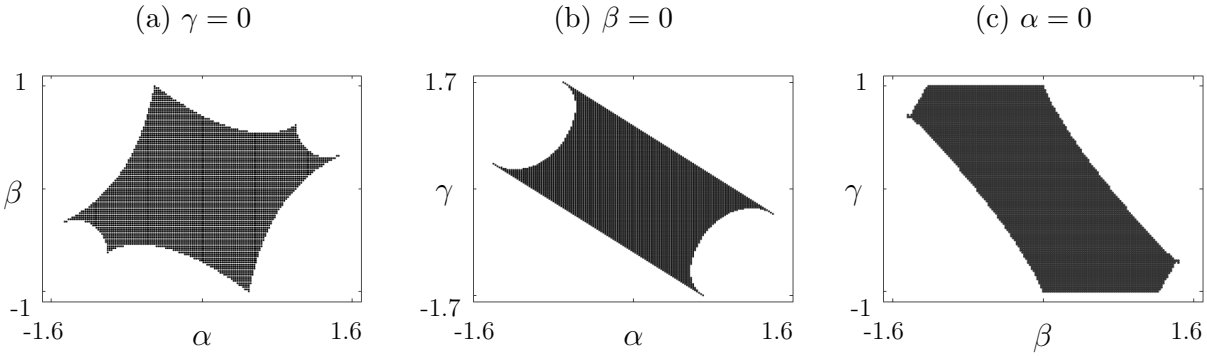

Figure XVII: *Varying domains of observability for the $n = 6$ model with two nonzero parameters. The rightmost plot is not cut off, but indeed an exact result.*

The domains of observability form (asymmetric) regions around zero in the parametric space, with their boundary consisting of so-called exceptional points (where the Hamiltonian, despite having real spectrum, ceases to be diagonalizable). The asymmetry of these plots serves as an inspiration to undertake a deeper numerical experiment with a single nonzero parameter. The results are summarized in tab. C for 4 different parameters.

	$n = 10$	$n = 30$	$n = 50$	$n = 100$
α_{crit}	1.0000	1.0000	1.0000	1.0000
β_{crit}	0.7129	0.7089	0.7082	0.7064
γ_{crit}	0.5228	0.5085	0.5027	0.5015
δ_{crit}	0.4535	0.3936	0.3913	0.3828

Table C: *Exceptional points for eq. 4.14 in n dimensions with a single nonzero parameter.*

With exception of the boundary parameter α, all the domains exhibit a shrinking behavior for growing n. Despite this fact, the shrinking rates fall down quickly, and one may conjecture that each p_{crit} approaches a certain nonzero limit for $n \to \infty$. This raises the possibility of existence of an appropriately defined infinite-dimensional limit, in complete analogy with eq. 4.4.

A related (and at this moment completely expected) question concerns another kind of limiting behavior. Assume again a family of operators with a single nonzero parameter, this time however having a fixed position with respect to the matrix center (instead of the boundary). As an example, choose the innermost (central) element c. The first three terms of the corresponding matrix family are then

$$H_2 = \begin{bmatrix} c & -1 \\ -1 & c \end{bmatrix} \qquad H_4 = \begin{bmatrix} & -1 & & \\ -1 & c & -1 & \\ & -1 & c & -1 \\ & & -1 & \end{bmatrix} \qquad H_6 = \begin{bmatrix} & -1 & & & & \\ -1 & & -1 & & & \\ & -1 & c & -1 & & \\ & & -1 & c & -1 & \\ & & & -1 & & -1 \\ & & & & -1 & \end{bmatrix} \tag{4.15}$$

One obvious advantage of taking this limit is, that the appropriate discrete limiting operation can be defined naturally as acting on $\ell^2(\mathbb{Z})$, whereas taking the limits in tab. C requires a more refined treatment. A numerical experiment analogical to the table above shows the values of exceptional points in tab. D

	$n = 10$	$n = 30$	$n = 50$	$n = 100$
c	1.0000	1.0000	1.0000	1.0000
c-1	0.4546	0.3678	0.3415	0.3467
c-2	0.5229	0.2583	0.2157	0.2133
c-3	0.7115	0.2355	0.1575	0.1572

Table D: *Exceptional points for eq. 4.15 in n dimensions with a single nonzero parameter. Interestingly, the innermost coupling behaves completely in the same way as the outermost one in tab. C.*

4.2.1 The universal metric

Inspired by the success enjoyed by the dual SSH Hamiltonian, we explore the possibility of constructing the universal metric for eq. 4.14 using once again the machinery of symbolic manipulations. Since our general Hamiltonian may be understood, up to a constant, as a perturbation of the discrete Laplacian

$$(\Delta_n)_{ij} = -\delta_{i,i+1} + 2\delta_{i,i} - \delta_{i+1,i} \tag{4.16}$$

(which is simplest possible discrete analogue of the Laplace operator, arising by second order finite difference discretization as in eq. 2.36) it may be fruitful to review the pseudometrics available for this operator. Their form useful for our later purposes turns out to be

$$\mathcal{P}^{(1)}(\Delta) = \begin{bmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & & 1 \end{bmatrix} \quad \mathcal{P}^{(2)}(\Delta) = \begin{bmatrix} 1 & & & \\ 1 & 1 & & \\ & 1 & 1 & \\ & & 1 & \end{bmatrix} \quad \mathcal{P}^{(3)} = \begin{bmatrix} & & 1 & \\ & 1 & & 1 \\ 1 & & 1 & \\ & 1 & & \end{bmatrix} \quad \mathcal{P}^{(4)} = \begin{bmatrix} & & & 1 \\ & & 1 & \\ & 1 & & \\ 1 & & & \end{bmatrix} \tag{4.17}$$

Since Δ is hermitian, the identity operator obviously belongs among admissible metrics, and so does the discrete parity operator $\mathcal{P}^{(n)}$. In sufficiently low dimensions, we can repeat this brute-force symbolic manipulation recipe for the general multiparametric Hamiltonian from eq. 4.14. In dimension four, this problem (depending on two parameters α, β) may be solved in full generality to reveal a sequence

$$\begin{aligned} \mathcal{P}^{(1)}(H) &= \begin{bmatrix} 1 & i\alpha & -\alpha(\alpha+\beta) & -i(\alpha(\alpha^2-\beta^2)-\beta) \\ -i\alpha & 1 & i\,(\alpha+\beta) & -\alpha\,(\alpha+\beta) \\ -\alpha\;(\alpha+\beta) & -i\,(\alpha+\beta) & 1 & i\alpha \\ i(\alpha(\alpha^2-\beta^2)-\beta) & -\alpha(\alpha+\beta) & -i\alpha & 1 \end{bmatrix} \\ \mathcal{P}^{(2)}(H) &= \begin{bmatrix} & & 1 & i(\alpha+\beta)\;\; \beta^2-\alpha^2 \\ & 1 & & 1 \quad\; i(\alpha+\beta) \\ -i(\alpha+\beta) & & 1 & \\ \beta^2-\alpha^2 & -i(\alpha+\beta) & 1 & \end{bmatrix} \\ \mathcal{P}^{(3)}(H) &= \begin{bmatrix} & & 1 & \mathrm{i}\alpha \\ & 1 & \mathrm{i}\beta & 1 \\ 1 & -\mathrm{i}\beta & 1 & \\ -\mathrm{i}\alpha & 1 & & \end{bmatrix} \qquad \mathcal{P}^{(4)}(H) = \begin{bmatrix} & & & 1 \\ & & 1 & \\ & 1 & & \\ 1 & & & \end{bmatrix} \end{aligned} \tag{4.18}$$

For large n, the general matrix elements are too complicated to be written explicitly. However, eq. 4.18 enables us to formulate a useful and simple ansatz, which may be expressed in a unified form for any dimension. The k-th matrix elements should again occupy just $n+1-k$ of its antidiagonals. The explicit dependence of the remaining elements is not specified, they are however required to be either purely real or purely imaginary, depending on their position (as expressed in fig. XVIII for $n = 6$)

When analyzing any model belonging to eq. 4.14, this ansatz may be readily applied to greatly reduce the arbitrariness of the undetermined metric. In particular, these considerations may be extended from the boundary interaction in eq. 4.3 to arbitrary single nonzero parameter, as demonstrated by examining the result for β

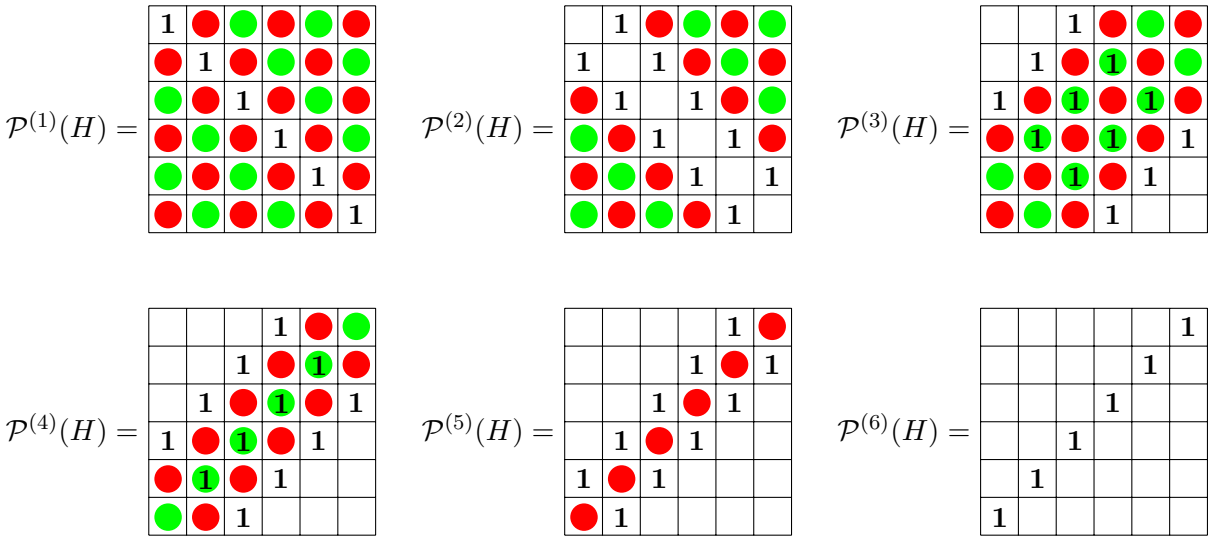

Figure XVIII: *A general ansatz for the pseudometrics of eq. 4.14 for any parameter values, depicted for $n = 6$. Red dots stand for imaginary entries, green dots for real entries, ones for the actual value 1.*

$$P_4^1(H_\beta) = \begin{bmatrix} 1 & & & \mathrm{i}\beta \\ & 1 & i\beta & \\ & -i\beta & 1 & \\ -\mathrm{i}\beta & & & 1 \end{bmatrix} \quad P_4^2(H_\beta) = \begin{bmatrix} & 1 & i\beta & -(i\beta)^2 \\ 1 & & 1 & i\beta \\ -i\beta & 1 & & 1 \\ -(i\beta)^2 & -\mathrm{i}\beta & 1 & \end{bmatrix}$$
$$P_4^3(H_\beta) = \begin{bmatrix} & & 1 & \\ & 1 & \mathrm{i}\beta & 1 \\ 1 & -\mathrm{i}\beta & 1 & \\ & 1 & & \end{bmatrix} \quad P_4^4(H_\beta) = \begin{bmatrix} & & & 1 \\ & & 1 & \\ & 1 & & \\ 1 & & & \end{bmatrix} \tag{4.19}$$

which in principle admits, due to its simplicity, the possibility of large-dimensional analytic discussion completely analogous to eq. 4.13. Although we do not pursue the general case here, the message is clear: in order to obtain closed-form pseudometrics, the interaction does not need to be constrained to the boundary.

The core of our present discussion lies in the introduction of yet another model, which remains apparently unnoticed in the literature. This model is notable for exhibiting a full-lattice interaction, meaning that all the parameters in eq. 4.14 are nonzero. It can be seen already from the $n = 4$ formulas, that maximum simplicity is achieved by choosing the parameters in an alternating fashion

$$\alpha = -\beta = \gamma = -\delta = \dots \tag{4.20}$$

A Hamiltonian with this precise choice of parameters shall be denoted H_a. The exceptional nature of this model indeed manifests itself when computing the pseudometric explicitly (using the provided ansatz in a convenient manner). The results of these computations are summarized in fig. XIX

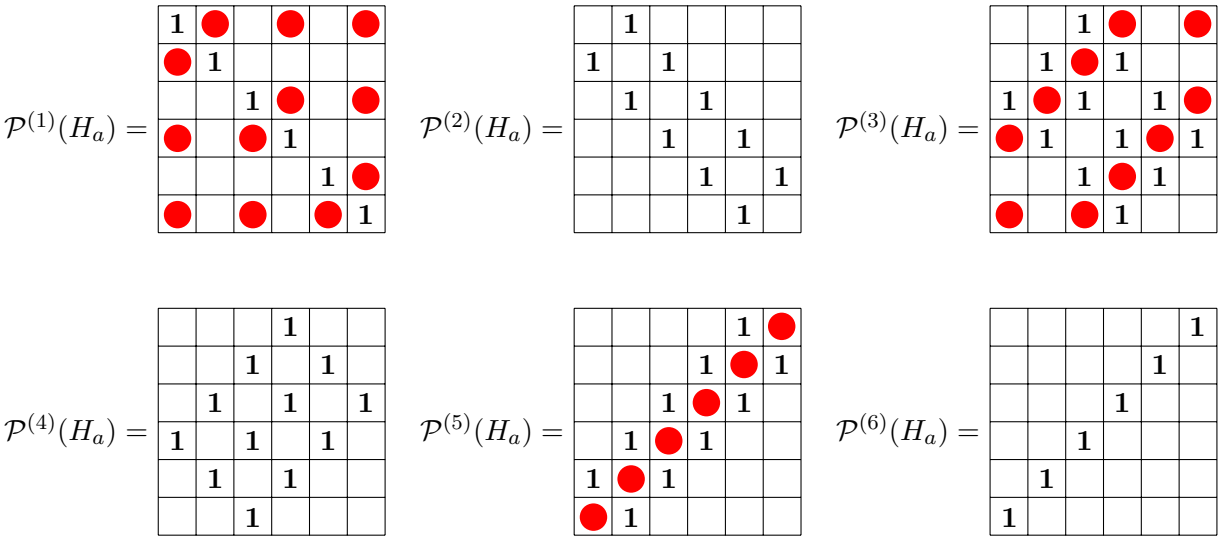

Figure XIX: *Matrix entries for $n = 6$ Hamiltonian of eq. 4.20, red dots standing for $\pm i\alpha$.*

The exceptionally friendly character of our interaction may be seen in the complete triviality of the even-numbered pseudometrics in each sequence, and also in the occurrence of just a single nontrivial matrix element $i\alpha$. Consequently, we may drop two-color notation from above, and denote this nontrivial element by a simple red dot.

We have reached the goal we were looking for: a successful construction of the pseudometrics for a special case of eq. 4.18, which surpasses the previously examined toy models (e.g. [112]) both in sparsity and simplicity of the resulting pseudometric elements. Our choice of Hamiltonian stems from the attempt to provide a general treatment to various finite-dimensional operators with complex interactions scattered in the literature. To this end, we complement the numerical experiment of previous section by its counterpart for full-lattice interactions.

	$n = 10$	$n = 30$	$n = 50$	$n = 100$
$\alpha = -\beta = \gamma = -\delta = \ldots$	0.2934	0.1015	0.0623	0.0316
$\alpha = \beta = \gamma = \delta = \ldots$	0.1413	0.0185	0.0073	0.0018

Table E: *Critical values (exceptional points) for 2 different full-lattice Hamiltonians of varying dimension n.*

The domains of observability are in orders of magnitude smaller that for single-site interactions, and have a clearly defined zero limit as $n \to \infty$. While these results complement nicely the single-site interactions discussed earlier, many problems in this direction remain unresolved. In this direction, it may be worth studying either general complex zero-range interactions (instead of purely complex ones), or switching attention to finite-range interactions, which would however most likely produce a number of new obstacles to overcome. The latter subject is so important, that we close this chapter with a short example of a model from finite-range class.

4.3 Beyond zero-range models

Even though zero-range Hamiltonians constitute a major portion of quantum-mechanical models, one is often forced to allow interactions of longer range in order to describe interesting physical phenomena. One such phenomenon is the Fano resonance [113], a type of resonance manifested by an asymmetric resonance line-shape. The general mechanism behind such resonance is the interference between two scattering processes, one in the continuous spectrum and the other being an excitation of a discrete state.

One of the simplest Hamiltonians exhibiting the Fano resonance is the lattice Fano-Anderson model [114, 115]. The underlying lattice can be taken as one-dimensional and doubly infinite. In other words, the Hamiltonian shall be assumed to act on the space $\ell^2(\mathbb{Z})$. It may be expressed in the second-quantized form as

$$H = -\sum_{n\in\mathbb{Z}\setminus\{1\}} a_{n-1}^\dagger a_n + g\left\{d_1^\dagger a_0 + d_2^\dagger a_0 + d_1^\dagger a_1 + d_2^\dagger a_1\right\} + h.c. \tag{4.21}$$

The sites d_1 and d_2 describe alternative channels for propagation of particles through the origin. These channels are coupled to the non-interacting Hamiltonian through the control parameter g, which shall be assumed to remain sufficiently small. A schematic picture of the Fano-Anderson model near the origin is depicted in fig. XX

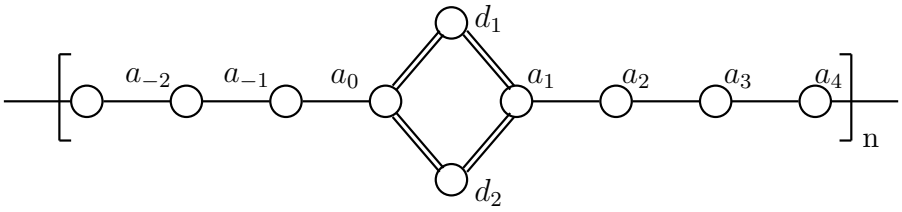

Figure XX: *Scheme of the Fano-Anderson Hamiltonian from eq. 4.21.*

In the following, we shall restrict attention to finite truncations of this Hamiltonian. While the truncated model can be no longer used to describe resonances and scattering phenomena, it is still suitable for description of certain physical scenarios. One example is a discrete quantum graph, modeling a (finite) network made from ultra-thin materials [116]. This approach was taken also in [111, 117], with results very similar to the truncated Fano-Anderson model.

In [118], a $\mathcal{PT}$-symmetrization of the Fano-Anderson system was suggested, with a gain-loss term localized in the center of the lattice, $H_I = i\gamma d_1^\dagger d_1 - i\gamma d_2^\dagger d_2$. Note that although the Fano-Anderson Hamiltonian is not tridiagonal, it is still a quadratic system and might be again represented in terms of $n \times n$ matrices instead of the usual Fock matrices of dimension $2^n \times 2^n$. The resulting Hamiltonian and a starting point of our considerations is

$$H = \begin{bmatrix} & -1 & & & & \\ -1 & & -g & -g & & \\ & -g & i\gamma & & -g & \\ & -g & & -i\gamma & -g & \\ & & -g & -g & & -1 \\ & & & & -1 & \end{bmatrix} \tag{4.22}$$

We wish to extend the method of pseudometric construction to the Fano-Anderson model. Since this means leaving the realm of tridiagonal models, the results can be expected to be considerably more involved. We illustrate all results for $n = 6$. For further discussion, it is helpful to divide the pseudometrics into three categories.

The first category contains $(n-1)/2$ pseudometrics independent on both g and γ, which demonstrate the trivial behavior of the Hamiltonian outside the bubble neighborhood of the origin. These metrics contain nonzero entries solely in their $(n-1)/2 \times (n-1)/2$ corner blocks, in our case

$$\mathcal{P}^{(1)} = \begin{bmatrix} & 1 & -1 & \\ 1 & & & -1 \\ & & & \\ -1 & & & 1 \\ & -1 & 1 & \end{bmatrix} \qquad \mathcal{P}^{(2)} = \begin{bmatrix} 1 & & & -1 \\ & 1 & -1 & \\ & & & \\ & -1 & 1 & \\ -1 & & & 1 \end{bmatrix} \tag{4.23}$$

These solutions can be naturally extended to larger dimensions. In general, they correspond to the chessboard solution of a free Laplacian on $(n-1)/2$ sites, completely analogous to eq. 4.17. In addition to this rather trivial family, we might construct a second (this time highly nontrivial) class of $(n-1)/2$ pseudometrics. The matrices of this family depend on both g and γ explicitly, with their form being to some extent compatible with the bubble shape of the original Hamiltonian. Explicitly for $n = 6$, we have

$$\mathcal{P}^{(3)} = \begin{bmatrix} 1 & & & & & 1 \\ 1 & & 2g & 2g & & 1 \\ & 2g & & -2i\gamma & 2g & \\ & 2g & 2i\gamma & & 2g & \\ 1 & & 2g & 2g & & 1 \\ & 1 & & & 1 & \end{bmatrix} \qquad \mathcal{P}^{(4)} = \begin{bmatrix} 1-4g^2 & & 2g & 2\,g & & 1-4g^2 \\ & & 1 & 2i\gamma g & -2i\gamma g & 1 & & \\ & 2g & -2i\gamma g & & -2\gamma^2 & -2i\gamma g & 2g & \\ & 2g & 2i\gamma g & -2\gamma^2 & & 2i\gamma g & 2g & \\ & & 1 & 2i\gamma g & -2i\gamma g & 1 & & \\ 1-4g^2 & & 2g & 2g & & 1-4g^2 \end{bmatrix} \tag{4.24}$$

The search is however not yet complete, it remains to reveal the form of two pseudometrics in order to get a complete family. One of them, as may be expected for a $\mathcal{PT}$-symmetric system, is again the discrete operator of parity $\mathcal{P}^{(5)}$. Note that of the five constructed pseudometrics, none are strictly positive. For $\gamma = 0$, the desired remaining (and positive) metric would be obviously the identity. The form of its $\gamma \neq 0$ counterpart, does not allow to isolate any reasonable extrapolating pattern, at least to our best knowledge. This may be seen as a first demonstration of the nontrivial nature of finite-range models, but at the same time as an open and physically highly relevant problem, encouraging further research in this direction.

Epilogue

It is not uncommon in physics for some important concepts or ideas to be initially neglected and eventually vanish into obscurity, only to be rediscovered many years later. A perfect example of this phenomenon is the very core of this thesis: quantum theory with non-hermitian observables. The possibility of using non-hermitian observables was pondered virtually since the first days of quantum mechanics by von Neumann [119] and Krein [120], and enjoyed a short *rennaissance* almost a generation later in the works of Dyson [121] and Dieudonné [122], to provide a small sample. Now, since nearly twenty years have passed since its last rediscovery in 1998, the theory seems to be firmly established in the physical literature.

Over the past years, the focus of researchers has gradually shifted from conceptual problems to applications of the theory. Probably the most successful of these applications, which is currently being unrivaled in terms of citations and press coverage, examines quasi-hermitian operators in classical optical systems [123, 124, 125, 126]. This is motivated by a formal similarity between the Schrödinger equation and some optical evolution equations, e.g. the Maxwell equations in paraxial approximation. As opposed to quantum physics, where quasi-hermitian theory provides a mere new mathematical formalism, the effects of non-hermicity are directly observable in optical systems. Among the newly observed phenomena, one of the most fascinating is definitely the recent possible realization of invisible metamaterials [127, 63].

In every physical theory, there is a strong need to establish at least a few exactly solvable models, which can be used as a reference point to further numerical or perturbative treatment. In comparison with ordinary quantum mechanics, quasi-hermitian theory is currently *in statu nascendi* in terms of availability and applicability of such models. The present thesis intends to help with filling the gaps in this direction. Its core lies in a thorough examination of a certain general class of finite-dimensional models and introduction of non-numerical construction patterns for the corresponding metrics.

Still, the thesis leaves unexplored many problems asking for further examination. The proper infinite-dimensional limits of discrete models in the spirit of eq. 4.3 and eq. 4.14 could probably be established for more general class of Hamiltonians. This could in principle lead to a substantial enlargement of the class of currently known solvable Hamiltonians. The same reasoning can be applied to the technique of $\mathcal{PT}$-symmetrizing known solvable hermitian Schrödinger operators, which has produced successful results for the square well potential [93, 128] as well as for the Coulomb Hamiltonian [89, 90]. Applying this technique to the whole class of Natanzon potentials, in the spirit of the works of Levai [129, 130, 131], could be strongly conjectured to produce some intriguing results.

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