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Pauli equation with non-Hermitian $\mathcal{PT}$-symmetric boundary condition

BACHELOR'S THESIS

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V Praze dne   Radek Novák

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Abstract:

The Pauli Hamiltonian in a bounded interval subjected to arbitrary $\mathcal{PT}$-symmetric Robin-type boundary conditions is investigated. It is introduced as an m-sectorial operator in a Hilbert space via quadratic form. We find the adjoint operator and conditions on various symmetries of the Hamiltonian using the quadratic form approach. We perform spectral analysis of the Hamiltonian and derive an implicit equation for the eigenvalues. These results are applied together with numerical analysis on several examples of boundary conditions and the metric operator is found for one of these examples.

Keywords: Pauli equation, Robin boundary conditions, scattering, PT-symmetry, spectral analysis, metric operator, quadratic form

Název: **Pauliho rovnice s nehermitovskými $\mathcal{PT}$-symetrickými hraničními podmínkami**
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Abstrakt:

V této práci je zkoumán Pauliho Hamiltonián na omezeném intervalu s obecnými $\mathcal{PT}$-symetrickými Robinovými hraničními podmínkami. Je zaveden jako m-sektoriální operátor na Hilbertově prostoru pomocí kvadratické formy. Přístupem přes kvadratickou formu nalézáme sdružený operátor a podmínky různých symetrií Hamiltoniánu. Provádíme spektrální analýzu Hamiltoniánu a odvozujeme implicitní rovnici pro vlastní čísla. Tyto výsledky pak aplikujeme spolu s numerickou analýzou na několik příkladů hraničních podmínek a nalézáme metrický operátor pro jeden z těchto příkladů.

Klíčová slova: Pauliho rovnice, Robinovy hraniční podmínky, PT-symetrie, spektrální analýza, metrika, kvadratická forma

Contents

Chapter 1

Introduction

Quantum mechanics is based, like other physical theories, on several axioms. One of these axioms states that the physical observables correspond to linear operators acting in a Hilbert space. It is also natural to require from these operators the reality of the points of the spectrum since these are the possible outcomes of a measurement. Traditionally, this is summarized in the condition that these operators have to be self-adjoint[1]. In the case of the Hamiltonian, this condition also ensures the unitary (probability preserving) time evolution of the system but it is not necessary for the reality of the spectrum. The non-self-adjoint operators, which are self-adjoint in a Hilbert space with a different scalar product, exist and this enables the creation of new alternative representations of quantum mechanics.

One of these attempts to use non-self-adjoint operators in quantum mechanics is the so-called $\mathcal{PT}$-symmetric quantum mechanics. Its main concern are the Hamiltonians exhibiting the simultaneous parity and time reversal symmetry. The interest in these Hamiltonians arose from the observation that many of them possess a real spectrum. Many such models were studied and it turned out that the key to the correct interpretation of these quantum systems is the finding of a bounded positive self-adjoint operator Θ, which can be used to define the new scalar product. However, this is in general a difficult task. In many models the metric operator cannot be found explicitly, the majority of known results provide just formal perturbative expansions. Therefore Krejčiřík, Bíla and Znojil developed in [21] a simple $\mathcal{PT}$-symmetric model where they found an explicit formula for the metric.

[1] We shall use in this text term self-adjoint which used usually in mathematical literature instead of its counterpart hermitian used in physical papers.

In this thesis we are interested in the role of spin in the model. It extends the model to a two dimensional matrix Hamiltonian and brings many classes of possible $\mathcal{PT}$-symmetric boundary conditions. An interesting feature of this extended model is its physical application - the scattering of a charged particle in a magnetic field can be described via this spectral problem [17].

This thesis is organized as follows. In the following Chapter 2 we bring a short overview of possible approaches to the $\mathcal{PT}$-symmetric quantum mechanics. In Chapter 3 we step by step approach the Hamiltonian, which is the main concern of this thesis. A special attention is paid to its scattering interpretation. Chapter 4 summarizes notions and theorems of spectral theory used in this thesis. It also brings a brief introduction to the theory of Sobolev spaces. Chapter 5 is dedicated to a rigorous mathematical definition of the Hamiltonian via quadratic form and finding the adjoint operator. The spectral analysis of the Hamiltonian is carried out in Chapter 6 and few examples of boundary conditions are studied. This section includes the numerical analysis of these examples. We conclude this thesis in Chapter 7, where we sum up our results and discuss their possible future extensions.

Chapter 2

$\mathcal{PT}$-symmetry

The idea of $\mathcal{PT}$-symmetry first emerged with the recognition that many non-self-adjoint Hamiltonians possess real spectrum. The family of Hamiltonians $H = -\Delta + x^2(\mathrm{i}x)^\varepsilon$, $\varepsilon \in \mathbb{R}_+$ acting in $L^2(\mathbb{R})$ was investigated firstly and it was discovered numerically that the eigenvalues of these Hamiltonians are entirely real, positive, and discrete [5]. This strange behaviour was attributed to the so-called $\mathcal{PT}$-symmetry of the Hamiltonian. This symmetry is often physically interpreted as parity-time reflection symmetry, however, there is deeper and more general mathematical background in this theory, which was developed during recent years. In this chapter we will take a closer look on three main approaches to the $\mathcal{PT}$-symmetry.

To avoid confusion, which could arise, we introduce a notion of D-self-adjointness. We say that an operator T is D-self-adjoint if for its adjoint operator holds

$$T^* = DTD \tag{2.1}$$

for some linear or antilinear operator D. This term is in literature used for a variety of operators D with different properties. It reduces in this text on the fulfillment of (2.1) and it will be always stressed out which properties of the operator D are required.

2.1 Antilinear symmetry

First way how to deal with $\mathcal{PT}$-symmetry is to introduce a general concept of the antilinear symmetry. This concept allows among others to work with the $\mathcal{PT}$-symmetric models in a general Hilbert space $\mathscr{H}$.

Definition 2.1.1. *Let T be a densely defined closed operator in $\mathscr{H}$. We say that T has an antilinear symmetry if there exists an antilinear bijective operator S and the relation*

$$TS\psi = ST\psi \tag{2.2}$$

holds for all $\psi \in \mathrm{D}(T)$.

In the framework of $\mathcal{PT}$-symmetric quantum mechanics the operator $\mathcal{PT}$ is chosen as the antilinear symmetry S. The operator $\mathcal{PT}$ is composed of two parts - the parity $\mathcal{P}$, representing spacial symmetry and acting in $L^2(\mathbb{R})$ space

$$(\mathcal{P}\psi)(x) := \psi(-x),$$

and the time-reversal $\mathcal{T}$, standing for a complex conjugation

$$(\mathcal{T}\psi)(x) := \overline{\psi(x)}.$$

Link between the time-reversal and the complex conjugation can be seen from the time-dependent Schrödinger equation

$$H\psi = \mathrm{i}\hbar\frac{\partial\psi}{\partial t}. \tag{2.3}$$

If we demand the system to be symmetric with respect to the time-reversal, the equation (2.3) should not change after the swap of t for $-t$. But the right-hand side changes the sign so we have to consider the effect of the complex conjugation operator to reproduce the form of the Schrödinger equation.

Both $\mathcal{P}$ and $\mathcal{T}$ satisfy relation $\mathcal{P}^2 = I, \mathcal{T}^2 = I$ and clearly commute with each other. Consequently, the operator $\mathcal{PT}$ is antilinear (since $\mathcal{P}$ is linear and $\mathcal{T}$ antilinear) and satisfies $(\mathcal{PT})^2 = I$. The property of $\mathcal{PT}$-symmetry of the Hamiltonian is then understood as fulfillment of the equation (2.2) for $S = \mathcal{PT}$.

Let us investigate further properties of the $\mathcal{PT}$ operator, in particular its spectrum and the influence it has on the spectrum of the Hamiltonian. We solve the equation

$$\mathcal{PT}\psi = \lambda\psi. \tag{2.4}$$

The equation (2.4) is transferred by application of operator $\mathcal{PT}$ and using the antilinearity of $\mathcal{PT}$ into the form $\psi = |\lambda|\psi$. Therefore the eigenvalues of $\mathcal{PT}$, $\lambda = \mathrm{e}^{\mathrm{i}\phi}$, are pure phases.

Assuming that E is an eigenvalue of the $\mathcal{PT}$-symmetric Hamiltonian H associated with an eigenvector ψ_E, we get, after simple algebraic manipulation,

$$H\mathcal{PT}\psi_E = \overline{E}\mathcal{PT}\psi_E,$$

so $\overline{E}$ is also an eigenvalue of H, associated with an eigenvector $\mathcal{PT}\psi_E$. The eigenvalue E is real if and only if the eigenvector ψ_E is $\mathcal{PT}$-symmetric, i.e. $\mathcal{PT}\psi_E = \psi_E$. We speak about *unbroken* $\mathcal{PT}$*-symmetry* if all eigenvectors of H are $\mathcal{PT}$-symmetric (and thus all eigenvalues are real). Or equivalently, if every eigenvector of H is an eigenvector of $\mathcal{PT}$. Conversely, if this does not apply for any eigenvector of H we speak about *broken* $\mathcal{PT}$*-symmetry*.

2.2 Pseudo-Hermiticity

It is evident from above that the $\mathcal{PT}$-symmetry is not a sufficient condition for the reality of the spectrum since the eigenvectors do not have to be $\mathcal{PT}$-symmetric. This is also supported by known $\mathcal{PT}$-symmetric models with a complex spectrum (e.g. previously mentioned model from [5] for $\varepsilon < 0$). Thus the search of properties of an operator which would ensure the reality of the spectrum began. The main interest was aroused by pseudo-Hermitian operators - many of the studied $\mathcal{PT}$-symmetric Hamiltonians showed this feature.

Definition 2.2.1 ([25])**.** *Let T be a densely defined linear operator in $\mathscr{H}$. T is called pseudo-Hermitian (or η-pseudo-Hermitian), if there exists an operator η with properties*

i) $\eta, \eta^{-1} \in \mathscr{B}(\mathscr{H})$,

ii) $T = \eta^{-1}T^*\eta$,

iii) $\eta = \eta^*$.

This concept came from the physical background and over time it became clear that there is an equivalent term in the mathematical literature - the J-self-adjointness in Krein spaces. Krein space $\mathscr{K}$ is a complex linear space endowed with a self-adjoint sesquilinear form $[\cdot\,,\cdot]$ (the so called indefinite inner product or indefinite metric). The positively definite scalar product $(\cdot\,,\cdot)$ can be defined and the fundamental symmetry J having properties $J = J^*$, $J^2 = I$ can be used to ensure the relation $[\phi, \psi] = (J\phi, \psi)$, $\phi, \psi \in \mathscr{K}$, between the former and the latter scalar product. Conversely, one can start with a Hilbert space with a positively definite scalar product and fundamental symmetry and define a Krein space.

The notion of an adjoint operator in Krein space is slightly different from the one in Hilbert space since it refers to the indefinite inner product. The Krein space adjoint $A^{[*]}$ of a densely defined linear operator A in $\mathscr{K}$ is defined by

$$[A\phi, \psi] = [\phi, A^{[*]}\psi] \quad \text{for } \phi \in \mathrm{D}(A), \psi \in \mathrm{D}(A^{[*]}) \tag{2.5}$$

where $\mathrm{D}(A^{[*]}) := \{\psi \in \mathscr{K} | [A\cdot\,, \psi] \text{ is continuous on } \mathrm{D}(A)\}$. The operator A is then called self-adjoint in Krein space if $A = A^{[*]}$. It follows from this property that $A^* = JAJ$ therefore this operator can be referred to as J-self-adjoint with respect to the fundamental symmetry J. For more details about the relation of the $\mathcal{PT}$-symmetry and the Krein spaces, the reader is referred to [24] and references therein.

To illustrate the relation between the pseudo-Hermiticity in Hilbert space and the J-self-adjointness in Krein space one can consider a η-pseudo-Hermitian operator A (i.e. $\eta A = A^*\eta$). Then we define Krein space using the self-adjoint form $[x, y]_\eta = (x, \eta y)$ and the fundamental symmetry $J = \eta\sqrt{\eta^2}^{-1}$. It can be easily verified that J satisfies all the requirements that it could be a conjugation operator in the Krein space. After further algebraic manipulation it can be verified that $JAJ = J^{[*]}$ and thus A is J-self-adjoint in this space [3]. In the scope of $\mathcal{PT}$-symmetric quantum mechanics is usually used the operator $\mathcal{P}$, it is therefore $\mathcal{P}$-self-adjointness.

A special class of pseudo-Hermitian operators are Quasi-Hermitian operators. Their importance was emphasized in [30] and since that time they hold an important place in $\mathcal{PT}$-symmetric quantum mechanics.

Definition 2.2.2 ([9])**.** *Let T be a densely defined linear operator in $\mathscr{H}$. T is called quasi-Hermitian, if there exists an operator Θ with properties*

- *i)* $\Theta, \Theta^{-1} \in \mathscr{B}(\mathscr{H})$,
- *ii)* $\Theta \geq 0$,
- *iii)* $T = \Theta^{-1}T^*\Theta$.

The operator Θ is called the metric operator or just the metric.

The main reason why the quasi-Hermitian operators are relevant to our purpose is the following: It was shown in [30] that for each irreducible set of quasi-Hermitean operator there exists a unique metric operator. With this operator it is possible to modify the scalar product

$$(\cdot\,,\cdot\,)_\Theta := (\cdot\,,\Theta\cdot\,). \tag{2.6}$$

In [30] it has been also proven the space with this metric is a Hilbert space. This enables a different approach to quantum mechanics - the suitable set of observables (non-self-adjoint but with real spectrum), for which a unique scalar product exists, is chosen, these observables are self-adjoint with respect to this scalar product and the calculations are then carried out in the Hilbert space defined by this scalar product.

The uniqueness is an important condition with regard to the statistical interpretation of quantum mechanics - it is impossible for a consistent quantum theory to yield multi-valent predictions. In other words, the expectation value of a physical observable could be different with respect to each non-unique scalar product. Another point of view is to regard the quasi-Hermitean operators as operators similar to the self-adjoint ones.

Theorem 2.2.3 ([4, Prop. 1])**.** *Let T be a quasi-Hermitian operator with metric operator Θ. Then T is similar to the self-adjoint operator H, $T = \rho H \rho^{-1}$, where $\rho = \sqrt{T}$.*

However, there still remains an open question - How to find the metric operator Θ? A partial answer for a finite-dimensional spaces can be found in [26, 25] and it is supplemented in [31]: Operator T is quasi-Hermitian if and only if its spectrum is real and it is diagonalizable (i.e. its eigenvectors form an bi-orthonormal basis). The operator Θ then has the form $\Theta = \sum_{j=0}^{n} c_j(\phi_j, \cdot)\phi_j$, where n is dimension of the Hilbert space, c_j are real positive constants and ϕ_j are eigenvectors of T^*. For infinite-dimensional spaces the general prescription for the metric operator exists only in special cases [21, 33, 28, 29] and most of the known examples of the metric are just approximative and expressed as the leading term of the perturbation series, e.g. in [6, 27].

2.3 C-self-adjointness

The substantial part of Hamiltonians studied in $\mathcal{PT}$-symmetric examples satisfies the relation $H^* = \mathcal{T}H\mathcal{T}$. It is not necessarily limited to $\mathcal{PT}$-symmetric models. This property found its counterpart in mathematic literature in the term of C-self-adjointness (not to be confused with the similar property associated with Krein spaces). The $\mathcal{PT}$-symmetry then can be understood as special case of C-self-adjointness.

Definition 2.3.1 ([10])**.** *An operator C defined on Hilbert space $\mathscr{H}$ is a conjugation operator, if for all $\phi, \psi \in \mathscr{H}$*

$$(C\phi, C\psi) = (\psi, \phi),$$
$$C^2\phi = \phi.$$

Definition 2.3.2 ([10]). *A densely defined operator T in $\mathscr{H}$ is said to be C-symmetric if $CTC \subset T^*$. T is complex-symmetric if it is C-symmetric for a conjugation operator C. T is said to be C-self-adjoint if $CTC = T^*$.*

The usefulness of this property is supported by the theorem proven in [7], which claims that the residual spectrum of these operators is empty. This significantly facilitates the spectral study of these non-self-adjoint operators. For more facts about complex symmetric operator the reader is referred to [11, 13, 14]

Chapter 3

Physical realisation

Let us consider a charged quantum particle of mass m and electric charge e. We will be interested in its interaction with a homogenous time-independent magnetic field. The Hamiltonian for a classical particle in a general electromagnetic field is given by

$$H = \frac{1}{2m}(\vec{p} - e\vec{A}(\vec{x}))^2 + e\phi(\vec{x}), \tag{3.1}$$

where $\vec{A}(\vec{x})$ is a vector potential and $\phi(\vec{x})$ is a scalar potential. Their relation to the vector of electric field intensity and vector of magnetic induction is $\vec{E} = -\mathrm{grad}\,\phi - \frac{1}{c}\frac{\partial \vec{A}}{\partial t}$ for the former and $\vec{B} = \mathrm{rot}\,\vec{A}$ for the latter. Using the correspondence principle, we can find the corresponding quantum Hamiltonian

$$\begin{aligned} H &= \frac{1}{2m}(\vec{P} - e\vec{A}(\vec{X}))^2 + e\phi(\vec{X}) \\ &= \frac{\vec{P}^2}{2m} - \frac{e}{m}(\vec{A}(\vec{X}).\vec{P}) + \frac{\mathrm{i}\hbar e}{2m}\mathrm{div}\,\vec{A}(\vec{X}) + \frac{e^2}{2m}|\vec{A}(\vec{X})|^2 + e\phi(\vec{X}). \end{aligned} \tag{3.2}$$

Capital $\vec{P}$ and $\vec{X}$ now denote the operators of momentum and position respectively,

$$\mathcal{P}_j\psi(\vec{x}) = -\mathrm{i}\hbar\frac{\partial}{\partial x_j}\psi(\vec{x}), \quad X_j\psi(\vec{x}) = x_j\psi(\vec{x}). \tag{3.3}$$

The index j assumes values $1, 2, 3$. If we now restrict ourselves to the case of homogenous time-independent magnetic field, we can choose potentials due to their gauge invariance so that $\phi(\vec{X}) = 0$ and $\vec{A}(\vec{X}) = \frac{1}{2}\vec{B} \times \vec{X}$. Hamiltonian (3.2) then takes form

$$H = \frac{\vec{P}^2}{2m} - \mu_0\vec{B}.\vec{L} + \frac{e^2}{8m}(\vec{B} \times \vec{X})^2, \tag{3.4}$$

where $\vec{L}$ is the vector of the angular momentum of the particle ($\vec{L} = \vec{X} \times \vec{P}$) and μ_0 is the magneton of the particle ($\mu_0 = \frac{e\hbar}{2m}$). The last term of this expression can be neglected for the usual values of magnetic induction (for more details on this step see [12]). We shall do this.

Hamiltonian (3.4) was in the dawn of the quantum theory experimentally verified on the Hydrogen atom. The theory claimed that the energy levels are going to split when the particle will be inserted into the magnetic field. This phenomenon was later named the Zeeman effect. In spite of the fact that the energy levels indeed split as it was predicted, the number of the new energy levels did not correspond with the predicted number and the energy of the ground state split as well as the other energy levels although it was not supposed to do so [18]. The corrections in the theory naturally followed with considerable support from the results of the Stern-Gerlach experiment. Another term depending on a discovered new internal property of particles, the spin, was added to the Hamiltonian.

Spin has nothing to do with the motion about the center of mass as it is in the macroworld. Characteristics of this intrinsic angular momentum were derived by means of the algebraic theory of spin in analogy with the algebraic theory of orbital angular momentum $\vec{L}$ [16]. Each type of particles has its own specific value of the spin. Thanks to these new degrees of freedom the description of the particle with a single wave function is not complete and therefore it is necessary to use functions with several independent components. Thus the operators need to be adjusted too - they become operator matrices. The operators not related to the magnetic field are for this purpose a multiplication of the identity matrix.

In the following text we are going to be concerned with particles with spin equal to $\frac{1}{2}$. Let us choose an electron as their representative. In the case of spin $\frac{1}{2}$ the wavefunctions (called also spinors) have two components and the operators are 2×2 matrices. The operator of spin $\vec{S}$ has three components

$$S_j = \frac{\hbar}{2}\sigma_j,$$

where σ_j are the Pauli spin matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -\mathrm{i} \\ \mathrm{i} & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}. \tag{3.5}$$

The modified Hamiltonian (3.4) now reads

$$H = \frac{\vec{P}^2}{2m} - \mu_0 \vec{B}.\vec{L} - 2\mu_0 \vec{B}.\vec{S}. \tag{3.6}$$

The added multiplicative constant 2 may look a little bit odd but there are reasons for adding it coming from quantum field theory. Reader interested in these reasons can find them e.g. in [15].

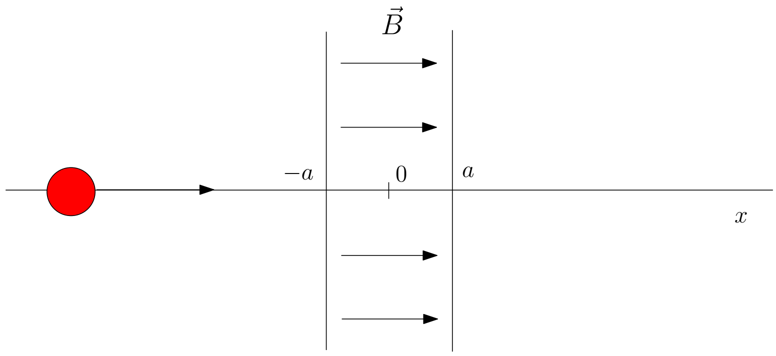

Figure 3.1: Electron passing through a magnetic field $\vec{B}$.

Assume that the electron flies into the homogenous magnetic field whose induction $\vec{B}$ is oriented in the direction of motion. We presume that the wavefunction is separable on three parts, each one depending only on one coordinate. We set the third coordinate axis in the direction of motion. We assume that the magnetic field is supported in the layer $\mathbb{R}^2 \times (-a, a)$. In this way, Hamiltonian for this direction will be diagonal, as the first term in Hamiltonian (3.6) is a multiplication of the identity operator, the second term disappears and the third one is composed of σ_3. We therefore arrive at

$$H = \begin{pmatrix} -\frac{\hbar^2}{2m}\Delta + \mu_0|B| & 0 \\ 0 & -\frac{\hbar^2}{2m}\Delta - \mu_0|B| \end{pmatrix} \tag{3.7}$$

defined on the Hilbert space $L^2((-a, a))$. We shall be interested in this thesis only in this one-dimensional scattering problem.

The Schrödinger equation for the spinor $\Psi = \binom{\psi_+}{\psi_-}$ reads

$$\begin{aligned} -\frac{\hbar^2}{2m}\psi_+'' + \mu_0|B|\psi_+ &= k^2\psi_+ \\ -\frac{\hbar^2}{2m}\psi_-'' - \mu_0|B|\psi_- &= k^2\psi_-, \end{aligned}$$

where k is a positive wave number. Thanks to vanishing of the potential outside of the interval $(-a, a)$ we have the asymptotic solutions

$$\Psi_i = \begin{pmatrix} c_1 \mathrm{e}^{\mathrm{i}kx} \\ c_2 \mathrm{e}^{\mathrm{i}kx} \end{pmatrix} + \begin{pmatrix} c_3 \mathrm{e}^{-\mathrm{i}kx} \\ c_4 \mathrm{e}^{-\mathrm{i}kx} \end{pmatrix} \tag{3.8}$$

for the in-coming wave and

$$\Psi_o = \begin{pmatrix} c_5 \mathrm{e}^{\mathrm{i}kx} \\ c_6 \mathrm{e}^{\mathrm{i}kx} \end{pmatrix} \tag{3.9}$$

for the out-coming wave. We introduced the complex constants $c_j, j = 1,2,3,4,5,6,$ which satisfy relations

$$|c_1|^2 + |c_2|^2 = 1,$$
$$|c_3|^2 + |c_4|^2 + |c_5|^2 + |c_6|^2 = 1.$$

The constant 1 determines just the normalization of the wavefunctions. This arrangement allows us to send in wave packets only with one component of the spinor and to study cases when the out-coming packet has only one component. We set further restriction by demanding the perfect transmission (i.e. $c_3 = c_4 = 0$).

If we employ this in the in-coming wave and request continuity of Ψ and Ψ' at the boundary $\pm a$, we reach the following non-linear problem

$$\begin{cases} -\frac{\hbar^2}{2m}\Psi'' + \begin{pmatrix} \mu_0|B| & 0 \\ 0 & -\mu_0|B| \end{pmatrix}\Psi &= k^2\Psi, \qquad \text{in } (-a,a), \\ \Psi'(\pm a) - \mathrm{i}k\Psi(\pm a) &= 0. \end{cases} \tag{3.10}$$

This non-linear problem can be studied via a linear spectral problem

$$\begin{cases} -\frac{\hbar^2}{2m}\Psi'' + \begin{pmatrix} \mu_0|B| & 0 \\ 0 & -\mu_0|B| \end{pmatrix}\Psi &= \mu(\alpha)\Psi, \qquad \text{in } (-a,a), \\ \Psi'(\pm a) - \mathrm{i}\alpha\Psi(\pm a) &= 0. \end{cases} \tag{3.11}$$

In this equation α is a real parameter and μ an eigenvalue depending on this parameter. We can then find energies of the perfect transmission states as $\mu(\alpha_*)$ for the points α_* which satisfy

$$\mu(\alpha_*) = \alpha_*^2. \tag{3.12}$$

In this manner we transformed the scattering problem at the interval $(-\infty, +\infty)$ to the spectral problem at the interval $(-a, a)$ with Robin boundary conditions. This type of boundary conditions has been appearing frequently in the course of the study of non-self-adjoint operators (i.e. [21, 20, 22, 7, 8]). These boundary conditions convert to Neumann boundary conditions for α tending to zero and to Dirichlet boundary conditions for α tending to infinity. In this thesis we will nevertheless consider more general cases of boundary conditions (see (5.2)) not necessarily with direct physical application. Owing to these boundary conditions the probability flow at the boundary points $\pm a$ does not disappear and therefore the non-self-adjointness can be interpreted as loss or gain of probability density at the boundary points. More details about the transforming scattering problems into $\mathcal{PT}$-symmetric spectral problems can be found in [17].

Chapter 4

Elements of the theory of sectorial forms

In the following paragraphs we will briefly summarize few basic properties of sectorial forms and Sobolev spaces which will be used in the subsequent chapters. We denote by $\mathscr{H}$ an arbitrary Hilbert space. Many of the following definitions and theorems can be further generalized, however, the presented forms are sufficient for our purposes. Let us start with the notion of a sesquilinear form.

Definition 4.0.1. *A complex valued function $t(\phi, \psi)$ defined for $\phi, \psi \in \mathrm{D}(t) \subset \mathscr{H}$ is called a sesquilinear form on $\mathscr{H}$ if it is antilinear in ϕ and linear in ψ. The function $t[\phi] := t(\phi, \phi)$ is called a quadratic form.*

The use of quadratic forms is convenient when we deal with Schrödinger operators (such as the Hamiltonian (3.7)) since they require less regularity of functions in its domain. Many differential operators with substantially different domains have quadratic forms with the same domain. In comparison with a similar problem for operators, it is not difficult to find the adjoint form, it is given by $t^*(\phi, \psi) := \overline{t(\psi, \phi)}, \mathrm{D}(t^*) := \mathrm{D}(t)$. A form t is said to be symmetric if $t(\phi, \psi) = t^*(\phi, \psi)$ for all $\phi, \psi \in \mathrm{D}(t) = \mathrm{D}(t^*)$. Knowing the adjoint form we can introduce the forms $\mathrm{Re}\, t := \frac{t+t^*}{2}$ and $\mathrm{Im}\, t := \frac{t-t^*}{2\mathrm{i}}$ called the real and the imaginary part of t, respectively. Let us note that neither $\mathrm{Re}\, t(\phi, \psi)$ nor $\mathrm{Im}\, t(\phi, \psi)$ are real-valued and thus have nothing to do with $\mathrm{Re}\,(t(\phi, \psi))$ and $\mathrm{Im}\,(t(\phi, \psi))$. They only satisfy the relations $\mathrm{Re}\, t[\phi] = \mathrm{Re}\,(t[\phi])$ and $\mathrm{Im}\, t[\phi] = \mathrm{Im}\,(t[\phi])$, which justify the notation.

We will further introduce the notion of numerical range which is important in various applications related to operators and forms in a Hilbert space.

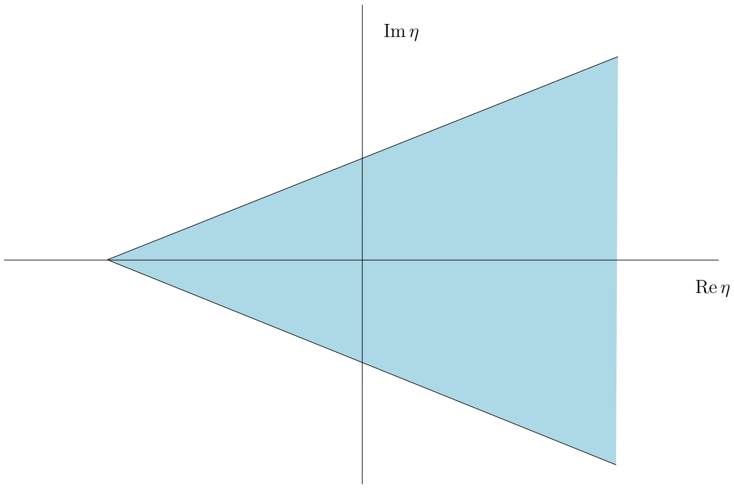

Figure 4.1: The numerical range $\Theta(t)$ of a sectorial form t is enclosed in a sector.

Definition 4.0.2. *Let t be a sesquilinear form in $\mathscr{H}$. We call the set $\{t[\phi]\,|\phi \in \mathrm{D}(t), \|\phi\| = 1\}$ the numerical range of t and denote $\Theta(t)$. Let T be an operator in $\mathscr{H}$. We call the set $\{(\phi, T\phi)\,|\phi \in \mathrm{D}(T), \|\phi\| = 1\}$ the numerical range of T and denote $\Theta(T)$.*

The numerical range need not to be open or closed, generally we can only say that it is a convex set in the complex plane.

4.1 Sectorial forms

For the symmetric forms, it is quite easy to establish in a very natural way the concept of boundedness from below since the quadratic form is real-valued. Our interest in forms bounded from below arises from the physical motivation to the problem studied in this thesis - the requirement of the ground state for the Hamiltonians considered in quantum mechanics is very customary and it has to be also fulfilled by their corresponding forms. In order to generalize this concept to the case of a nonsymmetric form we introduce the sectorial forms.

Definition 4.1.1 ([19])**.** *Let t be a sesquilinear form in the Hilbert space $\mathscr{H}$. The form t is said to be sectorially bounded from the left (or sectorial) if $\Theta(t)$ is a subset of a sector $\{\eta \in \mathbb{C}\,\big||\arg(\eta - \gamma)| \leq \theta, 0 \leq \theta < \frac{\pi}{2}, \gamma \in \mathbb{R}\}$ (see Figure 4.1), γ is called a vertex of t and θ a semi-angle.*

It follows from the definition that $\mathrm{Re}\, t \geq \gamma$ and $|\mathrm{Im}\, t[\phi]| \leq (\mathrm{Re}\, t[\phi] - \gamma)$ for $\phi \in \mathrm{D}(t)$. In other words, the real part of the form t is bounded from below and the numerical range is enclosed in a sector (see Figure 4.1). The numbers γ and θ are not uniquely determined by t. It is easy to see that the reduction of θ can be compensated by the reduction of γ.

To examine the sectoriality of the form using the perturbation theory we have to introduce the notion of relative boundedness which specifies the relation between two forms.

Definition 4.1.2 ([19])**.** *Let t be a sectorial form in $\mathscr{H}$. A form t' in $\mathscr{H}$ is said to be relatively bounded with respect to t (or t-bounded), if $\mathrm{D}(t') \supset \mathrm{D}(t)$ and*

$$|t'[u]| \leq a \|u\|^2 + b\,|t[u]| \tag{4.1}$$

where $u \in \mathrm{D}(t)$ and a,b are nonnegative constants.

We make the use of this property in the following theorem which gives us few properties of sums of forms.

Theorem 4.1.3 ([19, Thm. VI-1.33])**.** *Let t be a sectorial form in $\mathscr{H}$ and let t' be t-bounded with $b < 1$ in (4.1). Then $t + t'$ is sectorial. $t + t'$ is closed if and only if t is closed.*

In the light of this theorem we can divide the examined form into two parts and then consider the part t' just as a perturbation of the form t.

To introduce a term similar to the sectoriality of a form is not so simple for operators. In the following paragraph, we will step by step approach the notion of an m-sectorial operator.

Definition 4.1.4 ([10])**.** *A linear operator T acting in a Hilbert space $\mathscr{H}$ is said to be accretive if $\mathrm{Re}\,(\psi, T\phi) \geq 0$ for all $\phi \in \mathrm{D}(T)$, and quasi-accretive if $T + \alpha I$ is accretive for some $\alpha > 0$.*

Definition 4.1.5 ([10])**.** *A linear operator $\mathcal{T} \in \mathscr{C}(\mathscr{H})$ is said to be m-accretive if it satisfies*

$$\{\lambda \,|\, \mathrm{Re}\,\lambda < 0\} \subset \rho(T),$$

$$\|(T - \lambda I)^{-1}\| \leq \frac{1}{|\mathrm{Re}\,\lambda|} \qquad \textit{for} \quad \mathrm{Re}\,\lambda < 0.$$

If $T + \alpha I$ is m-accretive for some $\alpha > 0$, then T is said to be quasi-m-accretive.

Every m-accretive operator is accretive, hence its designation is justified. The notions of accretive and m-accretive operators are often used in problems concerned with the solvability of first- and second-order evolution equations and with differential equations of elliptic type. Hence these types of operators were deeply studied, many of their properties are known, but let us just state that if T is accretive then T^* is also accretive.

Definition 4.1.6 ([10])**.** *A linear operator T in a Hilbert space $\mathscr{H}$ is said to be sectorial if its numerical range lies in a sector $\{\eta \in \mathbb{C} \,\big|\, \operatorname{Re}\eta \geq \gamma, |\arg(\eta - \gamma)| \leq \theta, 0 \leq \theta < \frac{\pi}{2}, \gamma \in \mathbb{R}\}$. We say that T is m-sectorial if it is sectorial and quasi-m-accretive.*

The m-sectorial operators add to accretive operators further restrictions on the numerical range. They are often generated by second-order differential expressions with some boundary conditions. An important property of an m-sectorial operator is that it is closed.

It is known for a bounded form t that there exists a bounded operator T such that $t(\phi, \psi) = (\phi, T\psi)$. This theorem can be generalized to a densely defined, sectorial and closed form. The corresponding operator turns out to be not only closed and sectorial, as it would be expected, but even m-sectorial.

Theorem 4.1.7 ([19, Thm. VI-2.1], The first representation theorem)**.** *Let t be a densely defined, closed, sectorial sesquilinear form in $\mathscr{H}$. There exist an m-sectorial operator T such that*

i) $\mathrm{D}(T) \subset \mathrm{D}(t)$ *and* $t(u, v) = (u, Tv)$ *for every* $u \in \mathrm{D}(t)$ *and* $v \in \mathrm{D}(T)$*;*

ii) $\mathrm{D}(T)$ *is a core of t;*

iii) if $v \in \mathrm{D}(t), w \in \mathscr{H}$ and $t(u, v) = (u, w)$ holds for every u belonging to a core of t, then $v \in \mathrm{D}(T)$ and $Tv = w$.

The m-sectorial operator T is uniquely determined by the condition i).

An essential tool for investigating the spectrum of a closed operator is its resolvent. It captures the spectral properties of an operator in its analytic structure. Among other applications not related to this thesis belongs solving the inhomogenous Fredholm integral equations and finding the spectral decomposition of an operator.

Definition 4.1.8. *Let T be a closed operator. The set $\rho(T) := \{\lambda \in \mathbb{C} | (T - \lambda)^{-1}$ exists and is bounded$\}$ is called the resolvent set of T. The function R_T defined on $\rho(T)$ by $R_T(\lambda) := (T - \lambda)^{-1}$ is called the resolvent of T.*

The spectrum of on operator T is the set $\sigma(T) := \mathbb{C} \setminus \rho(T)$. The spectrum is always a closed set. It can be further separated into three parts - the point spectrum $\sigma_p(T)$ of such points λ (called also eigenvalues) that $T - \lambda$ is not injective, the continuous spectrum $\sigma_c(T)$ of such points λ that $T - \lambda$ is not surjective and $\operatorname{Ran}(T)$ is dense in $\mathscr{H}$ and the residual spectrum $\sigma_r(T)$ of such points λ that $T - \lambda$ is not surjective and $\operatorname{Ran}(T)$ is not dense in $\mathscr{H}$. All these sets are disjoint.

The investigation of properties of the resolvent R_T can lead to valuable information about the spectrum of T. The knowledge that the resolvent is compact for some λ turns out to be very useful. Then the resolvent is compact for all $\lambda \in \rho(T)$ and the spectrum of the operator T consists entirely of isolated eigenvalues with finite algebraic multiplicities. We can use the following theorem to verify the compactness of the resolvent.

Theorem 4.1.9 ([19, Thm. VI-3.4])**.** *Let s be a densely defined, closed sectorial form with $\operatorname{Re} s \geq 0$ and let S be the associated m-sectorial operator. Let t' be a t-bounded form satisfying (4.1) with $b < \frac{1}{2}$. Then $t = s + t'$ is also sectorial and closed. Let T be the associated m-sectorial operator. Then the resolvents R_S and R_T exists. If S has compact resolvent, the same is true of T.*

4.2 Sobolev spaces

Sobolev spaces are vector space whose elements are complex functions defined on domains in $\mathbb{R}^n$. Their partial derivatives are required to satisfy certain integrability conditions. The importance of Sobolev spaces lies in the fact that sometimes it is not sufficient to deal with the classical solutions of differential equations and it is necessary to work with distributions. We avoid in this text the general theory of Sobolev spaces and proofs of theorems and state just the notions relevant to this thesis. Interested reader can find more details on this theory in [1].

Let us start with the Hilbert space $\mathscr{H} := L^2((-a, a))$ with the norm $\|\cdot\|$. We call distribution every linear functional projecting smooth functions with a compact support contained in $(-a, a)$ into complex numbers. Every function f defined on $(-a, a)$ can be regarded as a distribution ϕ_f determined by the formula

$$\phi_f(g) := \int_{-a}^{a} f(x) g(x) \, \mathrm{d}x,$$

where g is a smooth function with a compact support in $(-a, a)$. The weak derivative $D^\alpha \phi$ for arbitrary $\alpha \in \mathbb{N}$ and distribution ϕ is defined by

$$(D^\alpha \phi)(g) := (-1)^\alpha \phi(D^\alpha g).$$

Let us now introduce the Sobolev space H^n. It is a special case of the more general Sobolev space $W^{n,p}$ for $p = 2$. We define the space

$$H^n((-a, a)) := \{f \in L^2((-a, a)) \,\big|\, D^\alpha f \in L^2((-a, a)), 0 \leq \alpha \leq n\}.$$

The norm is defined by the means of the formula

$$\|f\|_{n,2} := \left(\sum_{\alpha \leq n} \|D^\alpha f\|^2 \right)^{\frac{1}{2}}. \tag{4.2}$$

It can be proven that $H^2((-a, a))$ is a separable Hilbert space. It is obvious that it is imbedded in $L^2((-a, a))$ and it holds it is a dense subset. Due to one of the main results of the theory, the Sobolev imbedding theorem [1, Thm. 4.12], it holds that H^n is imbedded in the space consisting of functions having bounded, uniformly continuous derivatives up to order $n - 1$ on $[-a, a]$.

Chapter 5

Definition of the Hamiltonian

In this chapter we introduce the proper definition of the Hamiltonian (3.7) which arose from the physical motivation to the problem and we establish its basic properties. This Hamiltonian acts in the Hilbert space $\mathscr{H} := L^2((-a,a)) \otimes \mathbb{C}^2 \simeq L^2((-a,a);\mathbb{C}^2)$ on spinors $\Psi = \begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix}$. Scalar product in this space is defined as

$$(\Phi, \Psi) := \int_{-a}^{a} \overline{\Phi}^T(x)\Psi(x)\,\mathrm{d}x. \tag{5.1}$$

The corresponding norm is given as usual by $\|\Psi\| = \sqrt{(\Psi,\Psi)}$. The absolute value of spinor will be understood as $|\Psi(x)| = \sqrt{|\psi_+(x)|^2 + |\psi_-(x)|^2}$ for $x \in [-a,a]$. We impose Robin-type boundary conditions (RTBC),

$$\begin{aligned} \Psi'(a) + A\Psi(a) &= 0, \\ \Psi'(-a) - \overline{A}\Psi(-a) &= 0, \end{aligned} \tag{5.2}$$

where $A \in \mathbb{C}^{2\times 2}$,

$$A = \begin{pmatrix} p & q \\ r & s \end{pmatrix}, \qquad p,q,r,s \in \mathbb{C}. \tag{5.3}$$

This leads us to the definition of H

$$\begin{aligned} H\Psi &:= \begin{pmatrix} -\psi_+'' + c\psi_+ \\ -\psi_-'' - c\psi_- \end{pmatrix}, \\ \mathrm{D}(H) &:= \left\{ \Psi \in H^2((-a,a);\mathbb{C}^2) \,\middle|\, \begin{matrix} \Psi'(a) + A\Psi(a) = 0 \\ \Psi'(-a) - \overline{A}\Psi(-a) = 0 \end{matrix} \right\}, \end{aligned} \tag{5.4}$$

where $c := \mu_0|B| = \frac{e\hbar}{2m}|B|$. In order to simplify the form of the Hamiltonian, we used units in which $\hbar = 1$ and $m = 1/2$. We will keep this units for the rest of this thesis.

5.1 Definition via quadratic form

Equipped with the Hamiltonian, we can take a look how its associated sesquilinear form looks like. Starting from a general prescription for sesquilinear form $h(\Phi,\Psi)$ we obtain for all $\Psi \in \mathrm{D}(H)$ and $\Phi \in H^1((-a,a);\mathbb{C}^2)$

$$
\begin{aligned}
(\Phi, H\Psi) &= \int_{-a}^{a} \overline{\Phi}^T(x) H\Psi(x)\,\mathrm{d}x \\
&= \int_{-a}^{a} \Big(-\overline{\phi_+(x)}\psi_+''(x) + c\overline{\phi_+(x)}\psi_+(x) - \overline{\phi_-(x)}\psi_-''(x) - c\overline{\phi_-(x)}\psi_-(x)\Big)\,\mathrm{d}x \\
&= c(\phi_+,\psi_+) - c(\phi_-,\psi_-) - \int_{-a}^{a}\Big(\overline{\phi_+(x)}\psi_+''(x) + \overline{\phi_-(x)}\psi_-''(x)\Big)\,\mathrm{d}x \\
&= c(\phi_+,\psi_+) - c(\phi_-,\psi_-) - [\overline{\phi_+(x)}\psi_+'(x)]_{-a}^{a} - [\overline{\phi_-(x)}\psi_-'(x)]_{-a}^{a} \\
&\quad + \int_{-a}^{a}\Big(\overline{\phi_+'(x)}\psi_+'(x) + \overline{\phi_-'(x)}\psi_-'(x)\Big)\,\mathrm{d}x \\
&= (\Phi',\Psi') + c(\phi_+,\psi_+) - c(\phi_-,\psi_-) - \overline{\Phi}^T(a)\Psi'(a) + \overline{\Phi}^T(-a)\Psi'(-a).
\end{aligned}
$$

If we insert the boundary condition (5.2) into this equation, we get

$$
(\Phi, H\Psi) = (\Phi',\Psi') + c(\phi_+,\psi_+) - c(\phi_-,\psi_-) + \overline{\Phi}^T(a)A\Psi(a) + \overline{\Phi}^T(-a)\overline{A}\Psi(-a). \tag{5.5}
$$

Now we can move to the quadratic form by replacing Φ by Ψ in equation (5.5)

$$
\begin{aligned}
(\Psi, H\Psi) &= \|\Psi'\|^2 + c\|\psi_+\|^2 - c\|\psi_-\|^2 + \overline{\Psi}^T(a)A\Psi(a) + \overline{\Psi}^T(-a)\overline{A}\Psi(-a) \\
&= \|\Psi'\|^2 + c\|\psi_+\|^2 - c\|\psi_-\|^2 \\
&\quad + p|\psi_+(a)|^2 + q\overline{\psi_+(a)}\psi_-(a) + r\overline{\psi_-(a)}\psi_+(a) + s|\psi_-(a)|^2 \\
&\quad + \overline{p}|\psi_+(-a)|^2 + \overline{q}\overline{\psi_+(-a)}\psi_-(-a) + \overline{r}\overline{\psi_-(-a)}\psi_+(-a) + \overline{s}|\psi_-(-a)|^2.
\end{aligned} \tag{5.6}
$$

In order to see properties of the Hamiltonian (5.4) let us now start from the other end. We define sesquilinear form by the right-hand side of (5.5)

$$
\begin{aligned}
h(\Phi,\Psi) &:= (\Phi',\Psi') + c(\phi_+,\psi_+) - c(\phi_-,\psi_-) - \overline{\Phi}^T(a)\Psi'(a) + \overline{\Phi}^T(-a)\Psi'(-a), \\
\mathrm{D}(h) &:= H^1((-a,a);\mathbb{C}^2),
\end{aligned} \tag{5.7}
$$

without a priori knowing the operator from which it emerged. Notice that the boundary terms are well defined thanks to embedding of $H^1((-a,a);\mathbb{C}^2)$ in the space of uniformly continuous functions on $[-a,a]$ (see Chapter 4 for more details). It should be stressed out that form h has weaker requirements on the regularity of the functions than Hamiltonian H. Our first main goal is to show that this form is sectorial. To do this we prove the following auxiliary claim.

Lemma 5.1.1. *The inequality* $|\Psi(\pm a)|^2 \leq \frac{1}{2a}\|\Psi\|^2 + 2\|\Psi\|\|\Psi'\|$ *holds for all* $\Psi \in \mathrm{D}(h)$.

Proof. We make the following proof for $x = a$. The case of point $-a$ can be proven with a similar course of steps. We choose the auxiliary function η so that it complies

$$\eta(x) = \begin{cases} 0 & x \in (-\infty, -a) \\ \frac{x+a}{2a} & x \in [-a, a) \\ 1 & x \in [a, \infty) \end{cases}$$

Then it is possible to make the following estimate for $\Psi(a)$

$$\begin{aligned} |\Psi(a)|^2 &= \int_{-a}^{a} \frac{\mathrm{d}}{\mathrm{d}x}\left(\eta(x)|\Psi(x)|^2\right)\mathrm{d}x \\ &= \int_{-a}^{a} \eta'(x)|\Psi(x)|^2\,\mathrm{d}x + 2\int_{-a}^{a} \eta(x)|\Psi(x)||\Psi'(x)|\,\mathrm{d}x \\ &\leq \frac{1}{2a}\|\Psi\|^2 + 2\int_{-a}^{a} |\Psi(x)||\Psi'(x)|\,\mathrm{d}x \\ &\leq \frac{1}{2a}\|\Psi\|^2 + 2\|\Psi\|\|\Psi'\|. \end{aligned}$$

The Schwarz inequality $\int_{-a}^{a} |\Phi(x)||\Psi(x)|\,\mathrm{d}x \leq \left(\int_{-a}^{a} |\Phi(x)|^2\,\mathrm{d}x\right)^{\frac{1}{2}} \left(\int_{-a}^{a} |\Psi(x)|^2\,\mathrm{d}x\right)^{\frac{1}{2}}$ which holds for every $\Phi, \Psi \in \mathscr{H}$ was used in the last step. □

Let us now divide the form (5.7) into three parts:

$$\begin{aligned} h_1[\Psi] &= \|\Psi'\|^2 \\ h_2[\Psi] &= \mathrm{i}\,\mathrm{Im}\left(\overline{\Psi}^T(a)A\Psi(a) + \overline{\Psi}^T(a)\overline{A}\Psi(-a)\right) \\ h_3[\Psi] &= c\|\psi_+\|^2 - c\|\psi_-\|^2 + \mathrm{Re}\left(\overline{\Psi}^T(a)A\Psi(a) + \overline{\Psi}^T(-a)\overline{A}\Psi(-a)\right). \end{aligned} \tag{5.8}$$

This division is going to be used in the forthcoming theorems. Note that h_1 corresponds to Neumann Laplacian [10] and that $h_2[\Psi]$ is purely imaginary whereas $h_1[\Psi]$ and $h_2[\Psi]$ are real (see Chapter 4 for the definition of real and imaginary part of a form).

Theorem 5.1.2. *The form* h *defined by (5.7) is densely defined, closed and sectorial.*

Proof. The domain of h, $H^1((-a, a); \mathbb{C}^2)$, is dense in $\mathscr{H}$, hence h is densely defined. Using Lemma 5.1.1 we can carry out an upper bound on h_2 and h_3

$$\begin{aligned} |h_2[\Psi]| &\leq |A|(|\Psi(a)|^2 + |\Psi(-a)|^2) \leq \frac{|A|}{a}\|\Psi\|^2 + 4|A|\|\Psi\|\sqrt{h_1[\Psi]}, \\ |h_3[\Psi]| &\leq c\|\Psi\|^2 + \frac{|A|}{a}\|\Psi\|^2 + 4|A|\|\Psi\|\sqrt{h_1[\Psi]}, \end{aligned}$$

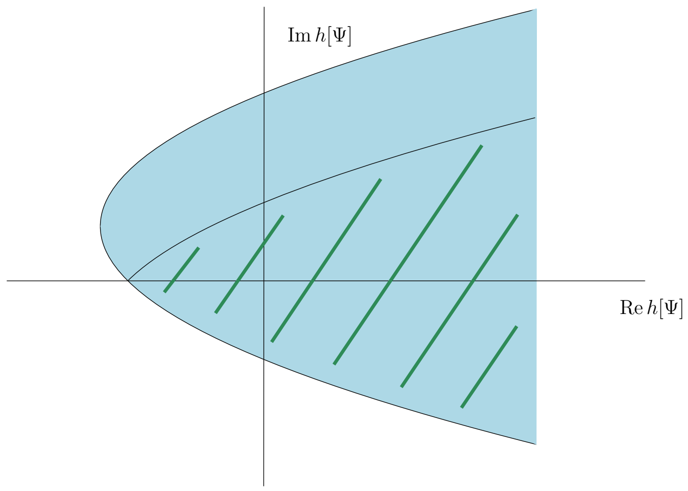

Figure 5.1: The numerical range $\Theta(h)$ of the sectorial form h is enclosed in a parabola. It can be further restricted with the use of Lemma 5.1.4.

where $|A| := |p| + |q| + |r| + |s|$. Putting these two estimates together we obtain

$$|(h_2 + h_3)[\Psi]| \leq 8|A|\|\Psi\|\sqrt{h_1[\Psi]} + \left(\frac{2|a|}{a} + c\right)\|\Psi\|^2$$
$$\leq 4|A|\varepsilon h_1[\Psi] + \left(\frac{4|A|}{\varepsilon} + \frac{2|a|}{a} + c\right).$$

In the last step we used the Young inequality $2ab \leq \varepsilon a^2 + \frac{b^2}{\varepsilon}$ which holds for all a and b real and $\varepsilon > 0$ for $a = \sqrt{h_1[\Psi]}$ and $b = \|\Psi\|$. This gives us that h_2+h_3 is h_1-bounded with the relative bound arbitrarily small since ε can be chosen arbitrarily small. h_1 corresponds to Neumann Laplacian in $\mathscr{H}$ and thus is densely defined, symmetric, positive and closed [10, Section IV.]. It follows easily from this that it is also sectorial. Therefore the form $h = h_1 + h_2 + h_3$ is according to Theorem 4.1.3 closed and sectorial. □

From Chapter 4 we know that the numerical range of a sectorial form is in a sector. However, in this case we can improve the estimate of the numerical range - instead of the sector we can enclose it in a parabola in the complex plane (see Figure 5.1). Thus the numerical range has much better behavior at the infinity.

Theorem 5.1.3. *The form (5.7) satisfies relation* $|\operatorname{Im} h[\Psi]| \leq C_1\sqrt{\operatorname{Re} h[\Psi] + C_2} + C_3$, *where* $C_1, C_2, C_3 > 0$.

Proof. Because the imaginary part of h is in fact h_2 we seek an upper bound containing square root of $h_1 + h_3$. We recall the estimate of h_2 and h_3 which we obtained in the proof of Theorem 5.1.2 considering we can normalize the function Ψ to 1

$$
\begin{aligned}
|h_2[\Psi]| &\le \frac{|A|}{a} + 4|A|\sqrt{h_1[\Psi]}, \\
|h_3[\Psi]| &\le c\|\Psi\|^2 + \frac{|A|}{a} + 4|A|\sqrt{h_1[\Psi]}.
\end{aligned}
$$

This estimate of h_2 is not yet what we desire, the real part of h is also composed of h_3. If we realise that the square root is an increasing function, we see that it is sufficient to proof

$$
h_1[\Psi] \le k_1\left(h_1[\Psi] + h_3[\Psi]\right) + k_2
$$

for some positive constants k_1 and k_2. To check this we carry on a lower estimate of $\operatorname{Re} h$

$$
\begin{aligned}
\operatorname{Re} h[\Psi] = (h_1 + h_3)[\Psi] &\ge h_1[\Psi] - \left(c + \frac{|A|}{a} + 4|A|\sqrt{h_1[\Psi]}\right) \\
&\ge (1-\varepsilon)h_1[\Psi] - \left(c + \frac{|A|}{a} + \frac{4|A|^2}{\varepsilon}\right) \\
&= \frac{1}{2}h_1[\Psi] - \left(c + \frac{|A|}{a} + 8|A|^2\right).
\end{aligned}
$$

In the last equality we set $\varepsilon = \frac{1}{2}$. This is exactly what we were trying to show. We can easily express h_1 from this equation

$$
0 \le h_1[\Psi] \le 2\operatorname{Re} h[\Psi] + 2\left(c + \frac{|A|}{a} + 8|A|^2\right). \tag{5.9}
$$

Altogether we obtained

$$
|\operatorname{Im} h[\Psi]| \le \sqrt{8}|A|\sqrt{\operatorname{Re} h[\Psi] + \left(c + \frac{|A|}{a} + 8|A|^2\right)} + \frac{|A|}{a}. \tag{5.10}
$$

Note that the square root is well defined thanks to the estimate (5.9). ☐

We also know from Lemma 5.1.4 that the numerical range is symmetric with respect to the real axis (the $\mathcal{PT}$-symmetry of the Hamiltonian is going to be presented in Chapter 6). Because the parabola is shifted, the numerical range is further restricted (see Figure 5.1).

Lemma 5.1.4. *Let $h(\phi, \psi) = (\phi, H\psi)$ for all $\phi \in \mathrm{D}(h), \psi \in \mathrm{D}(H)$, where H is $\mathcal{PT}$-symmetric. Then $\Theta(h)$ is symmetric with respect to the real axis.*

Proof. We recall from Chapter 2 that a $\mathcal{PT}$-symmetric operator satisfies $[H, \mathcal{PT}] = 0$ and that $(\mathcal{PT})^2 = I$. The numerical range $\Theta(h)$ is from definition given as the set of

$h[\psi] = (\psi, H\psi)$, where $\|\psi\| = 1$. Let us begin with such ψ. Then we can look at the point of $\Theta(h)$ associated with this vector

$$\begin{aligned} h[\psi] &= (\psi, H\psi) = (\mathcal{PT}\mathcal{PT}\psi, \mathcal{PT}\mathcal{PT}H\mathcal{PT}\mathcal{PT}\psi) = (\mathcal{PT}\tilde{\psi}, \mathcal{PT}H\tilde{\psi}) \\ &= (\mathcal{T}\tilde{\psi}, \mathcal{T}H\tilde{\psi}) = (H\tilde{\psi}, \tilde{\psi}) = \overline{(\tilde{\psi}, H\tilde{\psi})}, \end{aligned}$$

where we denoted $\tilde{\psi} := \mathcal{PT}\psi$. Our goal is to prove that $\operatorname{Re} h[\psi] - \mathrm{i}\operatorname{Im} h[\psi]$ also lies in $\Theta(h)$. This is indeed satisfied when we use $\tilde{\psi}$

$$\begin{aligned} \operatorname{Re} h[\tilde{\psi}] &= \frac{(\tilde{\psi}, H\tilde{\psi}) + \overline{(\tilde{\psi}, H\tilde{\psi})}}{2} = \frac{\overline{(\psi, H\psi)} + (\psi, H\psi)}{2} = \operatorname{Re} h[\psi] \\ \operatorname{Im} h[\tilde{\psi}] &= \frac{(\tilde{\psi}, H\tilde{\psi}) - \overline{(\tilde{\psi}, H\tilde{\psi})}}{2\mathrm{i}} = \frac{\overline{(\psi, H\psi)} - (\psi, H\psi)}{2\mathrm{i}} = -\operatorname{Im} h[\psi] \end{aligned}$$

□

We will show that sesquilinear form (5.7) defines the Hamiltonian (5.4). Using Theorem 4.1.7 we know that there exists an m-sectorial operator T defined via this form

$$\begin{aligned} T\Psi &:= \eta, \\ \mathrm{D}(T) &:= \{\Psi \in \mathrm{D}(h) \,|\, \exists \zeta \in \mathscr{H}, \forall \Phi \in \mathrm{D}(h), h(\Phi, \Psi) = (\Phi, \zeta)\}. \end{aligned} \tag{5.11}$$

By definition, T further satisfies the relation $h(\Phi, \Psi) = (\Phi, T\Psi)$ for all $\Phi \in \mathrm{D}(h)$ and $\Psi \in \mathrm{D}(T)$.

Theorem 5.1.5. *The Hamiltonian H defined by (5.4) equals to the operator T defined by (5.11).*

Proof. By integration by parts it can be directly shown that $H \subset T$. This is essentially the inverse process to that from which we originally derived the sesquilinear form.

It remains to prove $T \subset H$. The course of this proof is inspired by [19, Example VI.2.16]. In order to do so we come out of the Relation $h(\Phi, \Psi) = (\Phi, \zeta)$ which means

$$\int_{-a}^{a} \overline{\Phi}^T \zeta \,\mathrm{d}x = \int_{-a}^{a} \left(\overline{\Phi'}^T \Psi' + \overline{\Phi}^T C\Psi \right) \mathrm{d}x + \overline{\Phi}^T(a) A\Psi(a) + \overline{\Phi}^T(-a)\, \overline{A}\Psi(-a) \tag{5.12}$$

where $\Phi = \begin{pmatrix} \phi_+ \\ \phi_- \end{pmatrix} \in \mathrm{D}(h)$ and $\Psi = \begin{pmatrix} \psi_+ \\ \psi_- \end{pmatrix} \in \mathrm{D}(T)$ are functions of x and $C = \begin{pmatrix} c & 0 \\ 0 & -c \end{pmatrix}$ is a constant matrix. Let $z(x) := \int_{-a}^{x} (\zeta - C\Psi)\, \mathrm{d}y$. Then

$$\begin{aligned} \int_{-a}^{a} \overline{\Phi}^T (\zeta - C\Psi)\, \mathrm{d}x &= \int_{-a}^{a} \overline{\Phi}^T z' dx \\ &= \left[\overline{\Phi}^T z \right]_{-a}^{a} - \int_{-a}^{a} \overline{\Phi'}^T z \\ &= \overline{\Phi}^T(a) z(a) - \overline{\Phi}^T(-a) z(-a) - \int_{-a}^{a} \overline{\Phi'}^T z \,\mathrm{d}x. \end{aligned} \tag{5.13}$$

Putting equations (5.12) and (5.13) together yields

$$\int_{-a}^{a} \overline{\Phi'}^T \left(z + \Psi'\right) \mathrm{d}x + \overline{\Phi}^T(a)\left(A\Psi(a) - z(a)\right) + \overline{\Phi}^T(-a)\left(\overline{A}\Psi(-a) + z(-a)\right) = 0 \quad (5.14)$$

for every $\Phi \in \mathrm{D}(h)$ and $\Psi \in \mathrm{D}(T)$. For any $\Phi' \in L^2((-a,a);\mathbb{C}^2)$ such that $\Phi(x) = \int_{-a}^{x} \Phi'(x)\,\mathrm{d}x$, $\int_{-a}^{a} \Phi'(x)\,\mathrm{d}x = 0$ is valid, Φ lies in $\mathrm{D}(h)$ and satisfies $\Phi(a) = \Phi(-a) = 0$. It follows from equation (5.14) that $(z + \Psi') \perp \Phi'$ for this special choice of Φ. Thus $z + \Psi' \in \{1^{\perp}\}^{\perp} = \operatorname{span}\{1\}$ since

$$(1, \Phi') = \int_{-a}^{a} \Phi'(x)\,\mathrm{d}x = 0.$$

In other words $z + \Psi'$ equals to a constant k. Putting this into equation (5.14) we obtain by integration

$$\overline{\Phi}^T(a)\left(A\Psi(a) - z(a) + k\right) + \overline{\Phi}^T(-a)\left(\overline{A}\Psi(-a) + z(-a) - k\right) = 0.$$

Since $\Phi(a)$ and $\Phi(-a)$ can be any complex numbers when Φ varies over $\mathrm{D}(h)$, their coefficients must vanish. Together with the fact that $k = z(a) + \Psi'(a) = z(-a) + \Psi'(-a)$ we get

$$\begin{aligned} \Psi'(a) + A\Psi(a) &= 0, \\ \Psi'(-a) - \overline{A}\Psi(-a) &= 0. \end{aligned} \quad (5.15)$$

Further we can see that Ψ' is absolutely continuous and $\Psi'' = -z' = -\zeta + C\Psi \in L^2((-a,a),\mathbb{C}^2,dx))$. So for every $\Psi \in \mathrm{D}(T)$ it holds that Ψ and Ψ' are absolutely continuous and $\Psi'' \in L^2((-a,a),\mathbb{C}^2,dx)$. It further satisfies the boundary conditions (5.15). Ψ therefore belongs to $\mathrm{D}(H)$ and

$$T\Psi = \zeta = -\Psi'' + C\Psi.$$

These propertied directly show that $T \subset H$ since $\mathrm{D}(T) \subset \mathrm{D}(H)$ and $T\Psi = H\Psi$ for all $\Psi \in \mathrm{D}(T)$. □

5.2 Adjoint operator

Equipped with the First representation theorem we can take a look on the adjoint operator to Hamiltonian (5.4). Finding it can be in general difficult task but we opened a new way for finding it with its proper definition by sesquilinear form in Theorem 5.1.5.

Theorem 5.2.1. *The adjoint operator to Hamiltonian H defined by (5.4) is the operator H^* defined by*

$$
\begin{aligned}
H^*\Psi &= \begin{pmatrix} -\psi_+'' + c\psi_+ \\ -\psi_-'' - c\psi_- \end{pmatrix}, \\
\mathrm{D}(H^*) &= \left\{ \Psi \in H^2((-a,a);\mathbb{C}^2) \;\middle|\; \begin{matrix} \Psi'(a) + A^*\Psi(a) = 0 \\ \Psi'(-a) - A^T\Psi(-a) = 0 \end{matrix} \right\},
\end{aligned}
\tag{5.16}
$$

Proof. We can find the adjoint form to the form h from the definition

$$h^*(\Phi,\Psi) := \overline{h(\Psi,\Phi)} = (\Phi',\Psi') + c(\phi_+,\psi_+) - c(\phi_-,\psi_-) + \Psi(a)^T\overline{A}\,\overline{\Phi(a)} + \Psi^T(-a)A\overline{\Phi(-a)},$$

where $h(\Phi,\Psi)$ is the form (5.7). Basic properties of scalar product were used. The last two terms in this expression can be adjusted with basic matrix operations

$$
\begin{aligned}
\Psi(a)^T\overline{A}\,\overline{\Phi(a)} &= \overline{\Phi}^T(a)A^*\Psi(a), \\
\Psi^T(-a)A\overline{\Phi(-a)} &= \overline{\Phi}^T(-a)A^T\Psi(-a).
\end{aligned}
$$

after this algebraic manipulation, we obtain expression very similar to the original form (5.7). The only difference is the substitution of matrix A for matrix A^*. The expression for the adjoint operator follows from Theorem 4.1.7 and the proof of Theorem 5.1.5. □

With the knowledge of adjoint operator we can discuss when the Hamiltonian is D-self-adjoint for different choices of operator D. It turns out that impose conditions for the matrix A.

Proposition 5.2.2. *The Hamiltonian H is self-adjoint if and only if and only if $A = A^*$.*

Proof. We can directly compare both operators, we then see that they are identical when $A = A^*$. □

Proposition 5.2.3. *The Hamiltonian H is $\mathcal{P}$-self-adjoint if and only if $A = A^T$.*

Proof. Let us remind the relation satisfied by every $\mathcal{P}$-self-adjoint operator:

$$H^* = \mathcal{P}H\mathcal{P}.$$

It is not hard to verify that if $\Psi \in H^2((-a,a);\mathbb{C}^2)$ then also $\mathcal{P}\Psi \in H^2((-a,a);\mathbb{C}^2)$. Since the second derivative and the constant c are symmetric with respect to the parity, we have to check only the boundary conditions (5.2) and see how the vector $\mathcal{P}\Psi$ fits in:

$$
\begin{aligned}
\Psi'(a) + \overline{A}\Psi(a) &= 0, \\
\Psi'(-a) - A\Psi(-a) &= 0.
\end{aligned}
$$

By comparing this result with the original boundary condition (5.2) we see when the domains of H^* and $H\mathcal{P}$ coincide and we get the condition on $\mathcal{P}$-self-adjointnes $A = A^T$. □

Proposition 5.2.4. *The Hamiltonian H is $\mathcal{T}$-self-adjoint if $A = \overline{A}$.*

Proof. The proof is analogous to the proof of Proposition 5.2.3 □

Chapter 6

Spectral analysis

We approach the spectral analysis of Hamiltonian (5.4). Since this thesis is interested in operators having $\mathcal{PT}$-symmetry, let us check that our Hamiltonian fulfills this property.

Lemma 6.0.5. *The operator H defined by (5.4) is $\mathcal{PT}$-symmetric.*

Proof. We know from Definition 2.2 that H is $\mathcal{PT}$-symmetric if $[H, \mathcal{PT}] = 0$. This relation includes that for all $\Psi \in \mathrm{D}(H)$ holds that $\mathcal{PT}\Psi \in \mathrm{D}(H)$. We denote $\Phi(x) := (\mathcal{PT}\Psi)(x) = \overline{\Psi(-x)}$. With regard to properties of Sobolev spaces as mentioned in Chapter 4 we first must check that Φ, Φ' and Φ'' belong to $L^2((-a, a))$. This is trivially satisfied since it holds for Ψ. Φ should also satisfy RTBC (5.2) at $\pm a$. We shall check this for the point a

$$\begin{aligned}\Phi'(a) + A\Phi(a) &= -\overline{\Psi'(-a)} + A\overline{\Psi(-a)} \\ &= -\overline{\Psi(-a)} + \mathrm{Re}\,(A)\overline{\Psi(-a)} + \mathrm{i}\,\mathrm{Im}\,(A)\overline{\Psi(-a)} \\ &= \overline{-\Psi'(-a) + \mathrm{Re}\,(A)\Psi(-a) - \mathrm{i}\,\mathrm{Im}\,(A)\Psi(-a)} = 0.\end{aligned}$$

The proof for the point $-a$ is analogous. The statement now follows from the fact that the second derivative and the constant c commute with the operator $\mathcal{PT}$. □

The spectrum turns out to be discrete as it would be expected since our $\mathcal{PT}$-symmetric Hamiltonian is a differential operator on the compact interval. Nevertheless, there are few known examples of $\mathcal{PT}$-symmetric models with continuous spectrum [2, 7, 23].

Theorem 6.0.6. *The operator H defined by (5.4) is an operator with compact resolvent.*

Proof. According to Theorem (5.1.5), the operator H corresponds to the form (5.7). We recall the division of this form and the estimate carried out in the proof of the Theorem (5.1.2) which gives us that h_2+h_3 is h_1-bounded with the relative bound arbitrarily small.

It can be thus set smaller than $\frac{1}{2}$. Since h_1 corresponds to the Neumann Laplacian in $\mathscr{H}$ and thus is densely defined, closed and positive [10, Section IV.], it meets the requirements of Theorem 4.1.9. Because the Neumann Laplacian is an operator with compact resolvent, it follows from this theorem that H is an operator with compact resolvent. □

Corollary 6.0.7. *The spectrum of H consists entirely of isolated eigenvalues with finite algebraic multiplicities.*

We will try to broaden our knowledge about the point spectrum and try find the explicit form of the eigenvalues. Nevertheless, the latter is possible only in special cases of the RTBC (5.2), in the general case it turns out to be impossible. In general, our only way how to describe the eigenvalues is by means of an implicit equation.

Theorem 6.0.8. *The eigenvalues of H defined by (5.4) are determined by the equation*

$$\begin{aligned}
&\left((pk_+ - sk_-)^2 - (ps - qr + k_+k_-)^2\right)\cos\left(2a\left(k_- - k_+\right)\right)\\
&- \left((pk_+ + sk_-)^2 - (ps - qr - k_+k_-)^2\right)\cos\left(2a\left(k_- + k_+\right)\right)\\
&+ 2\left(pk_+ - sk_-\right)\left(ps - qr + k_+k_-\right)\sin\left(2a\left(k_- - k_+\right)\right)\\
&- 2\left(pk_+ + sk_-\right)\left(ps - qr - k_+k_-\right)\sin\left(2a\left(k_- + k_+\right)\right)\\
&+ 4qrk_+k_- = 0.
\end{aligned} \tag{6.1}$$

The corresponding eigenfunctions are

$$\Psi = \begin{pmatrix} A_+\cos(k_+x) + B_+\sin(k_+x) \\ A_-\cos(k_-x) + B_-\sin(k_-x) \end{pmatrix} \tag{6.2}$$

where $k_+ = \sqrt{\lambda + c}$ and $k_- = \sqrt{\lambda - c}$.

Proof. We are looking for the solution Ψ of the equation $H\Psi = \lambda\Psi$ in the form (6.2). Substituting this expression into the RTBC (5.2) we get equation

$$M\begin{pmatrix} A_+ \\ B_+ \\ A_- \\ B_- \end{pmatrix} = 0, \tag{6.3}$$

where $M \in \mathbb{C}^{4\times 4}$ is the matrix taking the form

$$\begin{pmatrix}
(p+\mathrm{i}k_-)\mathrm{e}^{\mathrm{i}ak_-} & (p-\mathrm{i}k_-)\mathrm{e}^{-\mathrm{i}ak_-} & q\mathrm{e}^{\mathrm{i}ak_+} & q\mathrm{e}^{-\mathrm{i}ak_+} \\
r\mathrm{e}^{\mathrm{i}ak_-} & \mathrm{e}^{-\mathrm{i}ak_-} & (s+\mathrm{i}k_+)\mathrm{e}^{\mathrm{i}ak_+} & (s-\mathrm{i}k_+)\mathrm{e}^{-\mathrm{i}ak_+} \\
(-\overline{p}+\mathrm{i}k_-)\mathrm{e}^{-\mathrm{i}ak_-} & (-\overline{p}-\mathrm{i}k_-)\mathrm{e}^{\mathrm{i}ak_-} & -\overline{q}\mathrm{e}^{-\mathrm{i}ak_+} & -\overline{q}\mathrm{e}^{\mathrm{i}ak_+} \\
-\overline{r}\mathrm{e}^{-\mathrm{i}ak_-} & -\overline{r}\mathrm{e}^{\mathrm{i}ak_-} & (-\overline{s}+\mathrm{i}k_+)\mathrm{e}^{-\mathrm{i}ak_+} & (-\overline{s}-\mathrm{i}k_+)\mathrm{e}^{\mathrm{i}ak_+}
\end{pmatrix}. \tag{6.4}$$

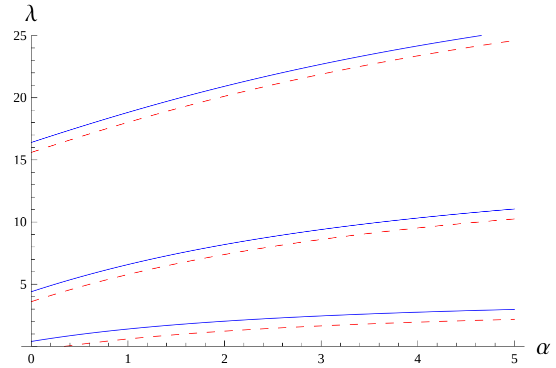

Figure 6.1: α-dependence of eigenvalues for $c = 0.4$, $a = \frac{\pi}{4}$ in Example a).

Nontrivial solution exists if and only if $\det(M) = 0$. This yields the equation (6.1). The eigenvectors are found by solving equation (6.3) with A_- (eventually with A_- and A_+) as a parameter. □

6.1 Examples of boundary conditions

In the following text we abandon the generality and examine few specific simple examples of RTBC (5.2) using Proposition 5.2.2 and Theorem 6.0.8. As the formulae simplify significantly, we continue in using notation $k_+ = \sqrt{\lambda + c}$ and $k_- = \sqrt{\lambda - c}$. Furthermore α always stands for a real positive parameter.

a)

$$A = \begin{pmatrix} \alpha & 0 \\ 0 & \alpha \end{pmatrix}$$

In this case we know from Proposition 5.2.2 that the eigenvalues are real. Equation (6.1) simplifies significantly and reads

$$\begin{aligned} &(2\alpha k_+ \cos(2ak_+) - (k_+^2 - \alpha^2)\sin(2ak_+)) \\ &(2\alpha k_- \cos(2ak_-) - (k_-^2 - \alpha^2)\sin(2ak_-)) = 0. \end{aligned} \tag{6.5}$$

The dependence of these eigenvalues on parameter α can be seen in Figure 6.1. Equation (6.5) is composed of the product of two terms. In order to satisfy the equation, at least one term in one of the two brackets must be equal to zero. The dashed line in the figure corresponds to the case when this condition is satisfied for the former, the full line for the latter. Due to separating both parts of the spinor in

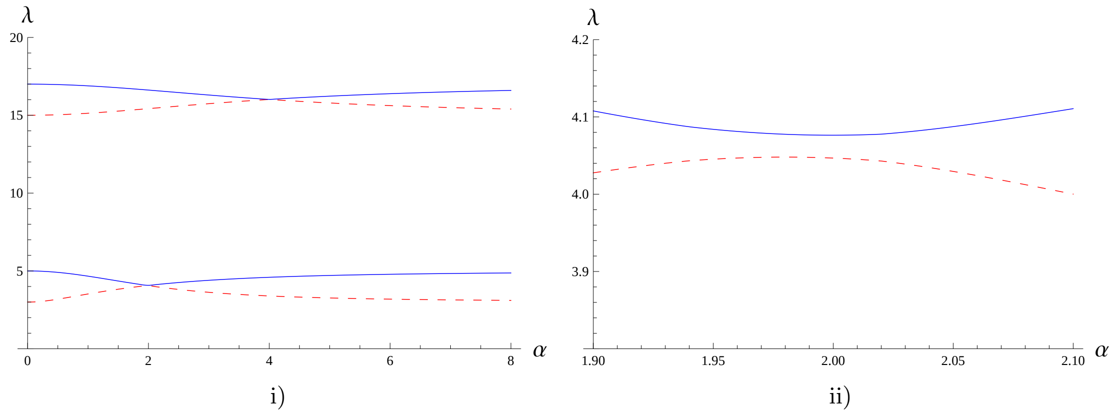

Figure 6.2: In i) α-dependence of eigenvalues for $c = 1$, $a = \frac{\pi}{4}$ in Example b). In ii) the detail of an avoided crossing of the first pair of eigenvalues.

the boundary condition, the final form of corresponding eigenvector depends on two parameters:

$$\Psi = \begin{pmatrix} A_+ \cos(k_+ x) + \frac{-\alpha\cos(ak_+)+k_+\sin(ak_+)}{k_+\cos(ak_+)+\alpha\sin(ak_+)} A_+ \sin(k_+ x) \\ A_- \cos(k_- x) + \frac{-\alpha\cos(ak_-)+k_-\sin(ak_-)}{k_-\cos(ak_-)+\alpha\sin(ak_-)} A_- \sin(k_- x) \end{pmatrix}.$$

b)

$$A = \begin{pmatrix} 0 & \mathrm{i}\alpha \\ -\mathrm{i}\alpha & 0 \end{pmatrix}$$

As well as in the previous example, we know in this one that the spectrum is real because the matrix defining boundary conditions is self-adjoint, cf. Proposition 5.2.2. The implicit equation for the eigenvalues now takes form

$$2\alpha^2 k_+ k_- (1 - \cos(2ak_+)\cos(2ak_-)) = -(k_+^2 k_-^2 + \alpha^4)\sin(2ak_+)\sin(2ak_-). \tag{6.6}$$

The dependence of these eigenvalues on parameter α can be seen in Figure 6.2. An interesting phenomenon in this figure is an approaching of a pair of eigenvalues and its subsequent moving back and slowly approaching to constant values. It should be noted that in the point of closest approach the two curves do not intersect. This avoided crossing holds for each pair of the eigenvalues. The exact form of the eigenvector for these eigenvalues depends solely on one parameter

$$\Psi = \begin{pmatrix} A\cos(k_+ x) + \frac{k_- k_+ \sin(ak_-)\sin(ak_+)+\alpha^2\cos(ak_+)\sin(ak_-)\tan(ak_-)}{k_- k_+ \cos(ak_+)\sin(ak_-)+\alpha^2\cos(ak_-)\sin(ak_+)} A\sin(k_+ x) \\ \frac{i\alpha\sin(ak_+)\left(k_- k_+ \sin(ak_+)+\alpha^2\cos(ak_+)\tan(ak_-)\right)}{k_-(k_- k_+ \cos(ak_+)\sin(ak_-)+\alpha^2\cos(ak_-)\sin(ak_+))} A\cos(k_- x) - \frac{i\alpha\cos(ak_+)}{k_-\cos(ak_-)} A\sin(k_- x) \end{pmatrix}.$$

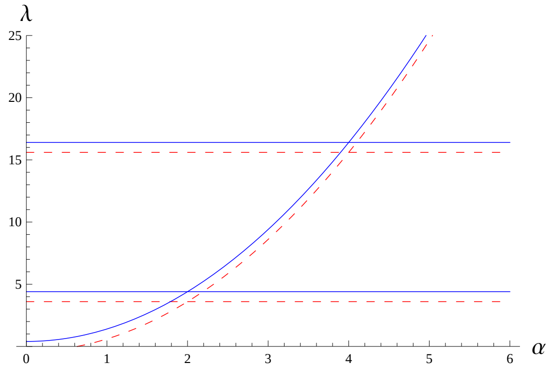

Figure 6.3: α-dependence of eigenvalues for $c = 0.4$, $a = \frac{\pi}{4}$, $\beta = 0$ in Example c).

c)

$$A = \begin{pmatrix} \mathrm{i}\alpha + \beta & 0 \\ 0 & \mathrm{i}\alpha + \beta \end{pmatrix}$$

Although the Hamiltonian satisfying these boundary conditions is not self-adjoint, we can still use the fact that they separate both parts of the spinor. Equation (6.1) can be rewritten in this case as

$$\begin{aligned} &\left(-2\beta k_- \cos(2ak_-) + (k_-^2 - \alpha^2 - \beta^2)\sin(2ak_-)\right) \\ &\left(-2\beta k_+ \cos(2ak_+) + (k_+^2 - \alpha^2 - \beta^2)\sin(2ak_+)\right) = 0. \end{aligned} \tag{6.7}$$

As a matter of fact, an eigenvalue problem corresponding to a very similar equation has been previously studied in [21] and in more detail in [22]. After a slight modification of results of [22] to our case the corresponding eigenfunctions read

$$\Psi = \begin{pmatrix} A_+ \cos(k_+ x) + \frac{k_+ \sin(ak_+) - (\mathrm{i}\alpha+\beta)\cos(ak_+)}{k_+ \cos(ak_+) + (\mathrm{i}\alpha+\beta)\sin(ak_+)} A_+ \sin(k_+ x) \\ A_- \cos(k_- x) + \frac{k_- \sin(ak_-) - (\mathrm{i}\alpha+\beta)\cos(ak_-)}{k_- \cos(ak_-) + (\mathrm{i}\alpha+\beta)\sin(ak_-)} A_- \sin(k_- x) \end{pmatrix}.$$

In further text we still suppose α and β real parameters. As we shall see, the spectrum has significantly different characteristics for different fixed values of parameter β.

The simplest case is $\beta = 0$. As it has been shown in [21] (for one dimensional case without magnetic field) and as it is seen from Figure 6.3 - one eigenvalue depends od parameter α quadratically and the others are constant. These eigenvalues can be expressed explicitly as

$$\lambda_{j,\pm} = \begin{cases} \alpha^2 \mp c, \\ \left(\frac{j\pi}{2a}\right)^2 \mp c. \end{cases} \tag{6.8}$$

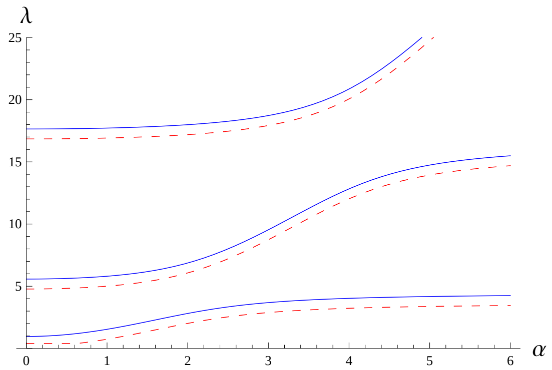

Figure 6.4: α-dependence of eigenvalues for $c = 0.4$, $a = \frac{\pi}{4}$, $\beta = 0.5$ in Example c).

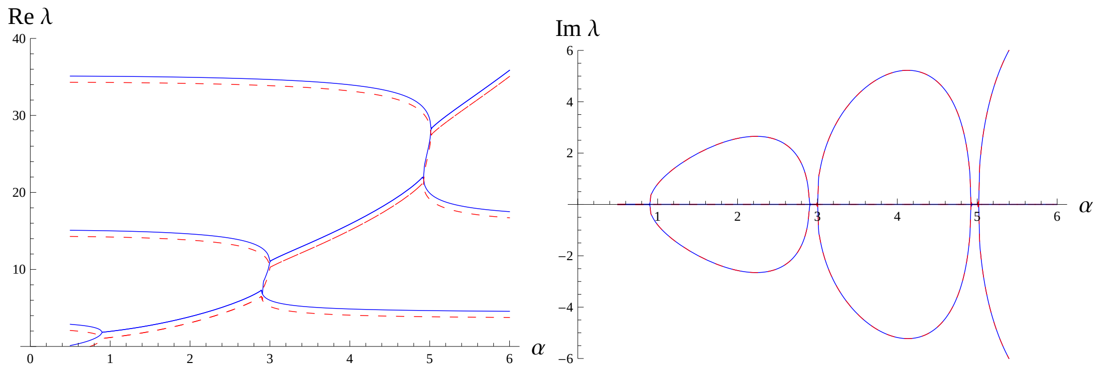

Figure 6.5: α-dependence of eigenvalues for $c = 0.4$, $a = \frac{\pi}{4}$, $\beta = -0.5$ in Example c).

Because equation (6.7) is composed of two terms, we can as in Example a) distinguish between cases when the first parenthesis is equal to zero and when this is true for the second one. Coherently with Example a), the dashed line in the figure corresponds with the case when the former case applies, the full line with the case when the latter applies.

The reality of the spectrum was proved for the case $\beta > 0$ in [22]. The Figure 6.4 shows dependance of these eigenvalues on parameter α. We can again observe the pairs of eigenvalues at a distance of $2c$.

However, the reality of spectra in the case when $\beta < 0$ is not guaranteed and indeed it is easily seen from the Figure 6.5 that complex conjugated pairs of eigenvalues appear and they have non-trivial imaginary part for large range of values of parameter α. This is manifested when two eigenvalues collide - then the imaginary part arises.

The situation when this pair of complex eigenvalues returns to real numbers can be also observed. It should be also noted that only one pair of complex conjugated eigenvalues occurs simultaneously in the spectrum [22].

This example of the boundary conditions can be easily interpreted physically in the scattering interpretation. We recall from Chapter 3 the boundary conditions in the equation (3.11), $\Psi'(\pm a) - \mathrm{i}\alpha\Psi(\pm a) = 0$. We consider adding two Dirac delta-interactions of strength $\beta \in \mathbb{R}$ located in the points $-a, a$. So the wavefunctions must further satisfy

$$\Psi'(-a_-) - \Psi'(-a_+) = \beta\Psi(-a),$$
$$\Psi'(a_-) - \Psi'(a_+) = \beta\Psi(-a).$$

It follows from the continuity of Ψ and Ψ' at the boundary $\pm a$ out more general example of boundary conditions.

d)

$$A = \begin{pmatrix} 0 & \mathrm{i}\alpha \\ \mathrm{i}\alpha & 0 \end{pmatrix}$$

This boundary conditions quite resemble those of case b). The equation determining the eigenvalues looks similar as well:

$$2\alpha^2 k_+ k_- (1 - \cos(2ak_+)\cos(2ak_-)) = (k_+^2 k_-^2 + \alpha^4)\sin(2ak_+)\sin(2ak_-). \tag{6.9}$$

That would draw one on the conclusion that the eingenvalues will also be real as the left-hand side of the equation contains trigonometric functions identical to those of the case b) and the right-hand side changed only the sign. This assumption would be wrong, since numerical simulations suggest that there appear complex eigenvalues (see Figure 6.6). The eigenvalues exhibit interesting feature - unlike the case c), this time only two eigenvalues meet and again divide after a while and no longer interact with the other eigenvalues. It is also apparent from other numerical calculations that only one pair of complex eigenvalues should appear simultaneously. The eigenvectors take a complex form similar to the one in case b)

$$\Psi = \begin{pmatrix} A\cos(k_+x) + \frac{k_-k_+\sin(ak_-)\sin(ak_+) - \alpha^2\cos(ak_+)\sin(ak_-)\tan(ak_-)}{k_-k_+\cos(ak_+)\sin(ak_-) - \alpha^2\cos(ak_-)\sin(ak_+)} A\sin(k_+x) \\ \frac{i\alpha\sin(ak_+)\left(k_-k_+\sin(ak_+) - \alpha^2\cos(ak_+)\tan(ak_-)\right)}{k_-(k_-k_+\cos(ak_+)\sin(ak_-) - \alpha^2\cos(ak_-)\sin(ak_+))} A\cos(k_-x) - \frac{i\alpha\cos(ak_+)}{k_-\cos(ak_-)} A\sin(k_-x) \end{pmatrix}.$$

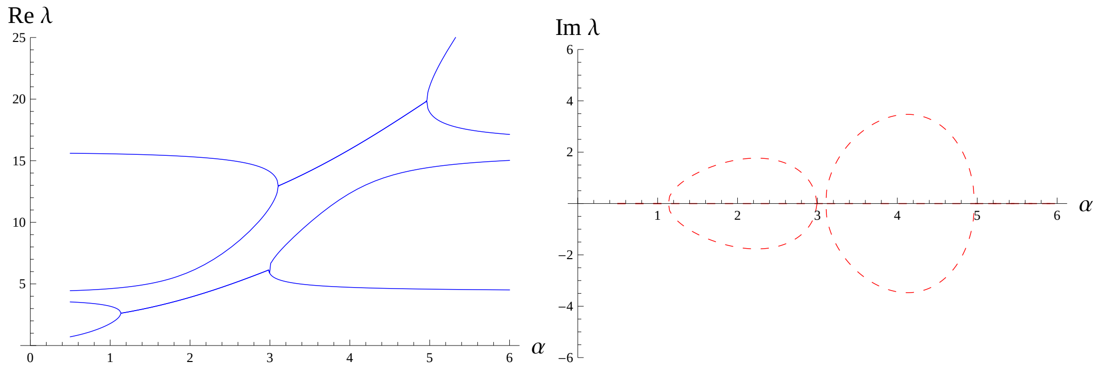

Figure 6.6: α-dependence of eigenvalues for $c = 0.4$, $a = \frac{\pi}{4}$, $\beta = -0.5$ in Example d).

6.2 Metric operator

In the end of this chapter we will take a look on the metric operator Θ_α for our spinor model as it was introduced in Section 2.2. We will consider only a simple example of the boundary conditions (5.2) with the matrix

$$A = \begin{pmatrix} \mathrm{i}\alpha & 0 \\ 0 & \mathrm{i}\alpha \end{pmatrix}.$$

We will make a use of the knowledge of metric operator θ_α for one dimensional case with the Hamiltonian h acting in the Hilbert space $L^2((-a,a))$

$$\begin{aligned} h\psi &:= -\psi'', \\ \mathrm{D}(h) &:= \left\{ \psi \in H^2((-a,a)) \,\middle|\, \psi'(\pm a) + \mathrm{i}\alpha\psi(\pm a) = 0 \right\}, \end{aligned}$$

where $\psi \in L^2((-a,a))$ and $\alpha \in \mathbb{R}$. The formula for the metric related to this Hamiltonian was firstly found in [21] and the elegant way of expressing this metric as

$$\theta_\alpha = I + K, \tag{6.10}$$

where K is an integral operator with kernel

$$\mathscr{K}(x,y) = \frac{1}{2a}\left(\mathrm{e}^{\mathrm{i}\alpha(y-x)} - 1\right) + \frac{\mathrm{i}\alpha}{2a}(y-x) - \frac{\alpha^2}{2a}xy + \frac{\alpha^2 a}{2} + \left(\mathrm{i}\alpha - \frac{\alpha^2}{2}(x-y)\right)\mathrm{sgn}(x-y), \tag{6.11}$$

was found in [32]. With the knowledge of eigenvalues (6.8) we can simplify the corresponding eigenvectors to the form

$$\begin{aligned} \Psi_n^+ &= \begin{pmatrix} \cos(k_n^+ x) - \mathrm{i}\frac{\alpha}{k_n^+}\sin(k_n^+ x) \\ 0 \end{pmatrix} \\ \Psi_n^- &= \begin{pmatrix} 0 \\ \cos(k_n^- x) - \mathrm{i}\frac{\alpha}{k_n^-}\sin(k_n^- x) \end{pmatrix}, \end{aligned} \tag{6.12}$$

where $k_n^\pm = \sqrt{\lambda_{j,\pm} \pm c}$. These vectors corresponding to different eigenvalues are clearly independent and therefore we can with the methods used in [21] find the metric expressed using the functions

$$\begin{aligned} \phi_0^\pm &= \sqrt{\frac{1}{2a}}\mathrm{e}^{\mathrm{i}\alpha x}, \\ \phi_n^\pm &= \sqrt{\frac{1}{2a}}\left(\cos(k_n^\pm x) + \mathrm{i}\frac{\alpha}{k_n^\pm}\sin(k_n^\pm x)\right), \qquad n \geq 1. \end{aligned}$$

The metric then takes the form of strongly convergent series

$$\begin{aligned} \Theta_\alpha &= \sum_{n=0}^{\infty} \begin{pmatrix} \phi_n^+ \\ 0 \end{pmatrix} \left(\begin{pmatrix} \phi_n^+ \\ 0 \end{pmatrix}, \cdot \right) + \sum_{n=0}^{\infty} \begin{pmatrix} 0 \\ \phi_n^- \end{pmatrix} \left(\begin{pmatrix} 0 \\ \phi_n^- \end{pmatrix}, \cdot \right) \\ &= \begin{pmatrix} \theta & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & \theta\alpha \end{pmatrix} \\ &= \theta_\alpha \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \end{aligned} \tag{6.13}$$

where $(\cdot,\cdot)$ is the scalar product (5.1) and θ_α is the one-dimensional metric (6.10). The metric Θ_α is bounded, symmetric, non-negative and satisfies the relation $H^*\Theta_\alpha\Psi = \Theta_\alpha H\Psi$ for all $\Psi \in \mathrm{D}(H)$. If we assume $\alpha \notin \frac{n\pi}{2a} \pm c)$ with $n \in Z \setminus \{0\}$ then the metric is positive. This can be immediately proven using the fact that these properties are already known for the one-dimensional metric θ_α in [21] and [32] (positivity). Peculiar feature of this metric is its form as a multiplication of the identity matrix and its dependence on the constant c. This constant does not appear in the explicit formula of the metric but only in the requirement on the positivity of the metric.

Chapter 7

Conclusions

In this thesis we investigated the influence of the magnetic field with Robin-type boundary conditions on a charged particle. The physically motivated Hamiltonian was introduced in a rigorous mathematical way via the quadratic form and further investigated. We proved that it is an m-sectorial operator with a compact resolvent. Main tool used during the investigation was the First representation theorem which was applied in this case of two dimensional vectors. The quadratic form approach enabled us to find easily the adjoint operator and conditions on self-adjointness, $\mathcal{P}$-symmetry, $\mathcal{T}$-symmetry and $\mathcal{PT}$-symmetry of the Hamiltonian, which restricted the boundary conditions.

Many types of boundary conditions were studied and few examples with purely real spectrum were found. Among these, there is an interesting self-adjoint example that connects both parts of the spinor. The numerical simulations suggest that if complex eigenvalues appear in the spectrum, there will always be simultaneously only one pair of complex conjugated eigenvalues. And finally for one of these boundary conditions we were able to find a metric operator which is just a multiplication of the identity matrix with the one-dimensional metric.

There still remain few open questions for further research. The list of the boundary conditions were not complete since we considered in this thesis only the $\mathcal{PT}$-symmetric boundary conditions. There are still undiscovered possibilities for $\mathcal{PT}$-symmetric boundary conditions with real spectrum and finding corresponding metric operator. At least but not last this thesis opened the way to further multidimensional generalisations of the original simple $\mathcal{PT}$-symmetric model.

Appendix A

Wolfram Mathematica source code

We state the source code of the Wolfram Mathematice software which was used for numerical calculations of α-dependencies of the points of the spectrum in Chapter 6 in Example d).

```
f[\[Lambda]_,\[Alpha]_,a_,c_] :=  4 \[Alpha]^2 Sqrt[-c+\[Lambda
    ]]
 Sqrt[c+\[Lambda]] Cos[a Sqrt[c+\[Lambda]]]^2 Sin[a Sqrt[-c+\[
    Lambda]]]^2
 +4 \[Alpha]^2 Sqrt[-c+\[Lambda]] Sqrt[c+\[Lambda]]
 Cos[a Sqrt[-c+\[Lambda]]]^2 Sin[a Sqrt[c+\[Lambda]]]^2
  +(c^2-\[Alpha]^4-\[Lambda]^2) Sin[2 a Sqrt[-c+\[Lambda]]]
   Sin[2 a Sqrt[c+\[Lambda]]]
Clear[eps,imax,m,a,alpha,w,w01,w1,w02,w2,w03,w3,w04,w4,r,s];
eps=0.001;imax=500;a=3.14/4; c=0.4; r=6;s=25;
w1=0.7; w2=3.6; w3=4.4; w4=15.5;
Table[alpha[i],{i,0,imax}];Table[w01[i],{i,0,imax}];Table[w02[i
    ],{i,0,imax}];
Table[w03[i],{i,0,imax}];Table[w04[i],{i,0,imax}];
For[i=0, i<imax+1, i++, alpha[i]=0.5+r*i/imax;
w1=w/.FindRoot[f[w,alpha[i],a,c]==0,{w,w1}];
w2=w/.FindRoot[f[w,alpha[i],a,c]==0,{w,w2}];
w3=w/.FindRoot[f[w,alpha[i],a,c]==0,{w,w3}];
w4=w/.FindRoot[f[w,alpha[i],a,c]==0,{w,w4}];
```

```
w01[i]=w1;w02[i]=w2;w03[i]=w3;w04[i]=w4;
w1=If[Abs[Re[w01[i]-w02[i]]]<eps && Abs[Im[w01[i]-w02[i]]]<eps,
   w1+0.5*I,w1];
w2=If[Abs[Re[w01[i]-w02[i]]]<eps && Abs[Im[w01[i]-w02[i]]]<eps,
   w2-0.5*I,w2];
w1=If[Abs[Re[w01[i]-w02[i]]]<eps && Abs[Im[w01[i]-w02[i]]]<eps,
   w1+0.5,w1];
w3=If[Abs[Re[w03[i]-w04[i]]]<eps && Abs[Im[w03[i]-w04[i]]]<eps,
   w3+0.5*I,w3];
w4=If[Abs[Re[w03[i]-w04[i]]]<eps && Abs[Im[w03[i]-w04[i]]]<eps,
   w4-0.5*I,w4];
w3=If[Abs[Re[w03[i]-w04[i]]]<eps && Abs[Im[w03[i]-w04[i]]]<500
   eps,w3+0.5,w3]]
Plot[{
Interpolation[Table[{alpha[i],Re[w01[i]]},{i,0,imax}]][x],
Interpolation[Table[{alpha[i],Re[w02[i]]},{i,0,imax}]][x],
Interpolation[Table[{alpha[i],Re[w03[i]]},{i,0,imax}]][x],
Interpolation[Table[{alpha[i],Re[w04[i]]},{i,0,imax}]][x]},
{x,0.5,r},PlotStyle->{{Blue},{Blue},{Blue},{Blue}},
AxesLabel->{Style[\[Alpha],16],Style["Re\[Lambda]",16]},
PlotRange->{0,s},AxesOrigin->{0,0}]
Plot[{
Interpolation[Table[{alpha[i],Im[w01[i]]},{i,0,imax}]][x],
Interpolation[Table[{alpha[i],Im[w02[i]]},{i,0,imax}]][x],
Interpolation[Table[{alpha[i],Im[w03[i]]},{i,0,imax}]][x],
Interpolation[Table[{alpha[i],Im[w04[i]]},{i,0,imax}]][x]},
{x,0.5,r},PlotStyle->{{Red,Dashing[Medium]},{Red,Dashing[Medium
   ]},
{Red,Dashing[Medium]},{Red,Dashing[Medium]}}, AxesLabel->{Style
   [\[Alpha],16],
Style["Im\[Lambda]",16]},PlotRange->{-6,6},AxesOrigin->{0,0}]
```

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