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DIPLOMOVÁ PRÁCE

**Teorie Kreinových prostorů pro nehermitovské
 \mathcal{PT} -symmetrické operátory**

**The Krein-space theory for non-Hermitian
 \mathcal{PT} -symmetric operators**

Posluchač: Bc. Jakub Železný

Školitel: Mgr. David Krejčířík, Ph.D.

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Jakub Železný

Název práce: **Teorie Kreinových prostou pro nehermitovské \mathcal{PT} - symmetrické operátory**

Abstrakt: V kvantové fyzice se pozorovatelné veličiny popisují Hermitovskými operátory. V případě tzv. quasi-Hermitovských operátorů je ale možné použít i nehermitovské operátory, protože tyto operátory jsou Hermitovské v Hilbertově prostou, jehož skalární součin je upravený pomocí tzv. metrického operátoru. Tato práce se zabývá jednoparametrickou třídou jednoduchých quasi-Hermitovských operátorů, zejména se zaměřuje na studium různých metrických operátorů a studium podobných Hermitovských operátorů.

Klíčová slova: kvantová fyzika, nehermitovské operátory, \mathcal{PT} -symmetrie, Kreinovy prostory, quasi-Hermitovské operátory

Title: **The Krein-space theory for non-Hermitian \mathcal{PT} -symmetric operators**

Author: Jakub Železný

Abstract: In quantum mechanics, observable quantities are usually described by Hermitian operators. However, it is also possible to use non-Hermitian operators, if these operators are the so-called quasi-Hermitian operators because these operators are Hermitian in a Hilbert space with scalar product modified using the so-called metric operator. We study a one-parametric class of simple quasi-Hermitian operators. We mainly focus on different forms of metric operators associated with these Hamiltonians and on similar Hermitian operators.

Key words: quantum physics, non-Hermitian operators, \mathcal{PT} -symmetry, Krein spaces, quasi-Hermitian operators

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Introduction

In quantum mechanics, observable quantities (usually called observables) are described by linear operators on some Hilbert space and possible outcomes of measurements correspond to points from their spectra. One of the basic axioms of quantum mechanics states that these operators are self-adjoint.¹ It is, however, possible to use non-self-adjoint operators as observables, if these operators are the so-called quasi-Hermitian operators ([36], [37] and also [24]). This is possible because these operators are self-adjoint in a Hilbert space with a scalar product modified using the so-called metric operator.

This formalism became relevant after discovery that non-self-adjoint Hamiltonians exhibiting certain symmetry (the so-called \mathcal{PT} -symmetry) often have real spectrum (see [8]). To interpret these Hamiltonians the so-called \mathcal{C} -operator is used to construct a new scalar product in which they are self-adjoint (see papers [9] or [32]).

The metric operator (or \mathcal{C} operator in case of \mathcal{PT} -symmetric operators) is crucial for interpreting the quasi-Hermitian operators. However the metric operator is usually complicated non-local operator, which cannot be found explicitly ([10], [11], [12], [31], [33]) and is usually expressed as leading terms in perturbative series. For this reason a new \mathcal{PT} -symmetric model was defined (see [21]), in which it is possible, due to the simplicity of the model, to find the metric operator explicitly and to treat the problem in a mathematically rigorous manner.

In this thesis we study the model further, we mainly focus on exploring different metric operators in this model and we calculate the corresponding self-adjoint operators. These operators are interesting because they might give a physical meaning to our model.

The work is organized as follows. In section 1 we give an introduction into the quasi-Hermitian operators in quantum mechanics and to \mathcal{PT} -symmetric quantum mechanics and we show how this theory can be put into the mathematical formalism of Krein spaces. In Section 2, we define the model and review some basic results about it from paper [20]. In Section 3 we study general form of the metric operator in the model. In Section 4 we give two examples of metric operators and in Section 5 we use them to find the corresponding similar self-adjoint operators.

1 Non-self-adjoint operators in quantum mechanics

Non-self-adjoint operators have been traditionally used in quantum mechanics to describe open quantum systems. Here we present a different way how non-self-adjoint operators can be used in quantum mechanics.

¹In physics, the term Hermitian is usually used instead. See Appendix A for more informations.

1.1 Mathematical description of quantum mechanics

In this section a brief introduction into mathematical description of quantum mechanics is given. For much more detailed discussion, we refer the reader to [13]. In quantum mechanics every system is associated with some Hilbert space and states of this system are represented by unit vectors from this Hilbert space. The observable quantities (called simply observables) are represented by self-adjoint operators on this Hilbert space and possible outcomes of the measurement of these observables are points from their spectra. Quantum mechanics is a probabilistic theory; it does not predict the result of an experiment with certainty, but it only predicts probabilities. If the system is in the state ψ and we perform a measurement of the observable A , the probability that the outcome of the experiment will lie in the Borel set Δ is given by

$$(\psi, E_A(\Delta)\psi), \quad (1.1)$$

where E_A is the spectral measure associated with the operator A . Specifically if λ_k is a simple eigenvalue and ψ_k the corresponding (normed) eigenfunction, the probability that the outcome of the experiment will be λ_k is

$$|(\psi, \psi_k)|^2. \quad (1.2)$$

If the outcome of the experiment is λ_k then after the measurement the system will be in state ψ_k . Mean value of the measurement of the observable A in the state ψ is given by

$$(\psi, A\psi). \quad (1.3)$$

Time evolution is governed by the Schrödinger equation

$$i\hbar \frac{d}{dt}\psi = H\psi, \quad (1.4)$$

where H is the observable corresponding to the energy of the system, the so-called Hamiltonian. For example the Hilbert space $L^2(\mathbb{R}^3)$ describes a spinless particle and the operators

$$\hat{x}_i\psi(x) = x_i\psi(x), \quad \hat{p}_i\psi(x) = -i\hbar \frac{\partial\psi(x)}{\partial x_i} \quad (1.5)$$

describe respectively i -th position and momentum. With proper domains these are self-adjoint operators. They satisfy the so-called canonical commutation relations

$$[\hat{x}_i, \hat{p}_j] = i\hbar. \quad (1.6)$$

If the particle is in the potential $V(x)$ then the Hamiltonian is

$$H\psi(x) = -\hbar^2\Delta\psi(x) + V(x)\psi(x). \quad (1.7)$$

It is important to understand why the self-adjoint operators are used. We will present three arguments:

1. One reason is that obviously the spectrum of operators, which describe observables, must be real. This is often the only reason given, but this is not sufficient reason because there are many non-self-adjoint operators, which have real spectrum, for example any operator similar to self-adjoint operator have real spectrum too. Another requirement is that the eigenvectors must be orthonormal. This must be so because it is an experimental result, that if we perform some measurement and then repeat the measurement immediately afterwards, the result will be the same.

Suppose we have an experiment, whose outcomes are $\{\lambda_j\}_{j=1}^{\infty}$ with corresponding states $\{\psi_j\}_{j=1}^{\infty}$. Note that it may happen that $\lambda_i = \lambda_k$. The states ψ_j must be orthonormal, we suppose that they form an orthonormal basis (or if they do not we can construct our Hilbert space such that they do form an orthonormal basis), then there exists a self-adjoint operator such that its eigenvalues are $\{\lambda_j\}_{j=1}^{\infty}$ and its eigenfunctions are $\{\psi_j\}_{j=1}^{\infty}$. It is given by:

$$A\psi = A \sum_{j=1}^{\infty} \alpha_j \psi_j \equiv \sum_{j=1}^{\infty} \alpha_j \lambda_j \psi_j, \quad (1.8)$$

where

$$\psi = \sum_{j=1}^{\infty} \alpha_j \psi_j \quad (1.9)$$

is the decomposition of ψ into the orthonormal basis $\{\psi_j\}_{j=1}^{\infty}$.

2. The expectation values must be real. If A is a bounded operator, then it follows from the condition

$$\forall \psi, \quad (\psi, A\psi) \in \mathbb{R} \quad (1.10)$$

that A is self-adjoint. In the case of unbounded operators, this is also true, if we suppose that $D(A) = D(A^*)$ (see [32, Appendix, Theorem 3]).

3. In the case of the Hamiltonian (which is usually the most important observable) there exists even stronger argument. Let $U(t_1, t_2)$ be a time evolution operator, i.e., an operator such that

$$U(t_1, t_2)\psi_{t_1} = \psi_{t_2}, \quad (1.11)$$

where ψ_{t_1} resp. ψ_{t_2} is a solution of Schrödinger equation at time t_1 resp. t_2 . We suppose our system is isolated, then $U(t_1, t_2) = U(t_1 - t_2)$. According to experiments, the time evolution conserves the scalar product of two states:

$$(\phi, \psi) = (U(t_1 - t_2)\phi, U(t_1 - t_2)\psi). \quad (1.12)$$

This is true even if the system is not isolated, but only closed. We will restrict ourselves, for simplicity, only to the case of isolated quantum systems. Then from (1.12) it follows that $U(t)$ must be a unitary operator for any t . If we add a reasonable assumption that $U(t)$ is for any t strongly continuous, then according to Stone's theorem (see Appendix A), there exist a self-adjoint operator A , such that

$$U(t) = e^{iAt}, \quad (1.13)$$

$$\frac{\partial}{\partial t} U(t)\psi_0 = iA\psi_t, \quad \forall \psi \in D(A). \quad (1.14)$$

The Hamiltonian is, therefore, equal to $-\hbar A$, which is a self-adjoint operator.

1.2 Quasi-Hermitian operators

It was shown in the previous section that using self-adjoint operators as observables in quantum mechanics is well physically motivated. However, as was proposed in paper [36], it is possible to use non-self-adjoint operators if we interpret them as self-adjoint operators in a different Hilbert space. This can be done in the case of the so-called quasi-Hermitian operators.

Definition 1.1. Let $\mathcal{A} = \{A_i\}_{i \in \mathcal{I}}$ be a set of densely defined linear operators on some Hilbert space \mathcal{H} and let there exist a bounded positive operator θ with bounded inversion, such that

$$A_i^* \theta = \theta A_i, \quad \forall i \in \mathcal{I}. \quad (1.15)$$

Then the set \mathcal{A} is called **quasi-Hermitian** and θ is called a **metric operator** (associated with the set \mathcal{A}).

Remark 1.2. We stress out that the precise meaning of relation (1.15) is the following

$$D(A_i^*) = \theta D(A_i), \quad (1.16)$$

$$A_i^* \theta \psi = \theta A_i \psi, \quad \forall \psi \in D(A_i). \quad (1.17)$$

Following theorems summarize properties of quasi-Hermitian operators. The first two were proven in [36], where, however, only bounded operators were considered. While this does not pose in principle any physical limitation because in experiments we can always measure bounded functions of unbounded observables, it is inconvenient from the practical point of view as operators in quantum mechanics are usually unbounded. We provide proofs valid even for unbounded operators. The proof of the second theorem is, more or less, a straightforward extension of the proof from [36].

Theorem 1.3. Let $\mathcal{A} = \{A_i\}_{i \in \mathcal{I}}$ be a quasi-Hermitian set on some Hilbert space \mathcal{H} . Then all operators A_i are self-adjoint in the Hilbert space \mathcal{H}_θ , which is the same as Hilbert space \mathcal{H} as a set, but is endowed with a different scalar product:

$$(\phi, \psi)_\theta \equiv (\phi, \theta\psi), \quad (1.18)$$

where (\cdot, \cdot) is a scalar product of the Hilbert space \mathcal{H} .

Theorem 1.4. Let $\mathcal{A} = \{A_i\}_{i \in \mathcal{I}}$ be a quasi-Hermitian set on some Hilbert space \mathcal{H} and let θ be some metric operator associated with this set. This metric operator is unique (up to a multiplicative factor) if and only if \mathcal{A} is irreducible when considered in \mathcal{H}_θ (see Appendix A).

Theorem 1.5. Let $\mathcal{A} = \{\tilde{A}_i\}_{i \in \mathcal{I}}$ be a set of quasi-Hermitian operators with metric operator θ and let ρ be a bounded operator with bounded inversion such that $\theta = \rho^*\rho$. Such operator always exists because we can choose $\rho = \sqrt{\theta}$. Then every \tilde{A}_i is similar to self-adjoint operator $A_i = \rho\tilde{A}_i\rho^{-1}$. Furthermore ρ is unitary if considered as

$$\rho : \mathcal{H}_\theta \rightarrow \mathcal{H}. \quad (1.19)$$

Remark 1.6. There exists infinitely many decompositions $\theta = \rho^*\rho$. This is because if ρ is a bounded operator with bounded inversion such that $\theta = \rho^*\rho$, then $\rho' = \rho U$ is also bounded operator with bounded inversion and $\theta = \rho'^*\rho'$, for any unitary operator U on \mathcal{H}_θ . Conversely if ρ_1, ρ_2 are bounded operators with bounded inversions, such that $\theta = \rho_{1,2}^*\rho_{1,2}$, then there exists a unitary operator U on \mathcal{H}_θ such that $\rho_1 = \rho_2 U$.

Proof of Theorem 1.3. $(\phi, \psi)_\theta$ is obviously a scalar product. Moreover it holds that:

$$m(\phi, \phi) \leq (\phi, \phi)_\theta \leq M(\phi, \phi), \quad (1.20)$$

where $m = \inf\{(\phi, \theta\phi) | \phi \in \mathcal{H}, \|\phi\| = 1\}$ and $M = \|\theta\|$. m must be positive because θ is positive and it must be strictly positive since otherwise 0 would lie in the spectrum of θ and θ^{-1} would not be bounded (see [13, Proposition 3.4.5]). Norms on \mathcal{H}_θ and \mathcal{H} are, therefore, equivalent so topologies on \mathcal{H}_θ and on \mathcal{H} are the same. From this it, among other things, follows that \mathcal{H}_θ is complete and \mathcal{H}_θ is, therefore, a Hilbert space.

Let A_i^\dagger denote the adjoint of A_i in the Hilbert space \mathcal{H}_θ . Vector ϕ lies in $D(A_i^\dagger)$ if and only if there exists a vector φ such that

$$(\phi, A_i\psi)_\theta = (\varphi, \psi)_\theta, \quad \forall \psi \in D(A_i). \quad (1.21)$$

This can be written as

$$(\theta\phi, A_i\psi) = (\theta\varphi, \psi), \quad \forall\psi \in D(A_i). \quad (1.22)$$

Therefore, ϕ lies in $D(A_i^\dagger)$ if and only if $\theta\varphi$ lies in $D(A_i^*)$:

$$D(A_i^\dagger) = \theta^{-1}D(A_i^*) = D(A_i), \quad (1.23)$$

and for $\phi \in D(A_i)$ (1.22) can then be rewritten as

$$(\varphi, \psi)_\theta = (A_i^*\theta\phi, \psi) = (\theta A_i\phi, \psi) = (A_i\phi, \psi)_\theta, \quad \forall\psi \in D(A_i). \quad (1.24)$$

Thus $A_i^\dagger = A_i$. □

Proof of Theorem 1.4. Let us first suppose that \mathcal{A} is irreducible and let θ, θ' be two different metric operators associated with \mathcal{A} . Then using relations

$$A_i^*\theta = \theta A_i, \quad (1.25)$$

$$A_i^*\theta' = \theta' A_i. \quad (1.26)$$

we can easily show that

$$A_i\theta'^{-1}\theta\phi = \theta'^{-1}\theta A_i\phi, \quad \forall\phi \in D(A_i). \quad (1.27)$$

Operator $\theta'^{-1}\theta$, therefore, lies in the commutant of \mathcal{A} . When considered on \mathcal{H}_θ , \mathcal{A} is an irreducible set of self-adjoint operators, so we can use Theorem A.5:

$$\theta'^{-1}\theta = cI \Leftrightarrow \theta = c\theta'. \quad (1.28)$$

Conversely assume that \mathcal{A} is reducible (on \mathcal{H}_θ). Let E be the projection from Definition A.3 and let $F = I - E$. Let α, β be any positive numbers and let $V = \alpha E + \beta F$. We will show that for any metric operator θ , $\theta' = \theta V$ is also a metric operator. θ' is bounded because θ and V are bounded. Since E and F are self-adjoint operators in \mathcal{H}_θ , they must satisfy:

$$E^*\theta = \theta E, \quad (1.29)$$

$$F^*\theta = \theta F, \quad (1.30)$$

and, therefore, also

$$V^*\theta = \theta V. \quad (1.31)$$

θ' is then self-adjoint:

$$\theta'^* = V^*\theta^* = \theta V = \theta'. \quad (1.32)$$

It is also positive because:

$$(\phi, \theta' \phi) = \alpha(E\phi, \theta E\phi) + \beta(F\phi, \theta F\phi) > 0. \quad (1.33)$$

The inversion of V is:

$$V^{-1} = \frac{1}{\alpha}E + \frac{1}{\beta}F, \quad (1.34)$$

which is a bounded operator, therefore θ'^{-1} is also bounded. We now have to show that θ' satisfies relations (1.15). We first show that $\theta'D(A_i) = D(A_i^*)$. It must hold that $VD(A_i) \subset D(A_i)$ because of property (A.9). To show that the converse relation also holds, let $\psi \in D(A_i)$. We can decompose ψ as

$$\psi = \psi_1 + \psi_2, \quad \psi_1 \in E\mathcal{H}, \quad \psi_2 \in F\mathcal{H}. \quad (1.35)$$

Since $E\psi = \psi_1$ and $F\psi = \psi_2$, both ψ_1 and ψ_2 must lie in $D(A_i)$. Then also any their linear combination lies in $D(A_i)$. We set:

$$\phi = \frac{1}{\alpha}\psi_1 + \frac{1}{\beta}\psi_2 \quad (1.36)$$

Then $V\phi = \psi$ so $VD(A_i) = D(A_i)$ and, therefore, $\theta'D(A_i) = D(A_i^*)$. Using decomposition (1.35) we can easily show that

$$A_i V \psi = V A_i \psi, \quad \forall \psi \in D(A_i). \quad (1.37)$$

Using this relation

$$A_i^* \theta' \phi = A_i^* \theta V \phi = \theta A_i V \phi = \theta' A_i \phi, \quad \forall \psi \in D(A_i). \quad (1.38)$$

□

Proof of Theorem 1.5. Let $\phi, \psi \in \mathcal{H}$

$$(\rho\phi, \rho\psi) = (\phi, \rho^* \rho\psi) = (\phi, \psi)_\theta \quad (1.39)$$

and ρ is, therefore, unitary. ϕ lies in $D(A_i)$ if and only if there exists $\varphi \in \mathcal{H}$ such that

$$(\phi, A_i \psi) = (\phi, \psi), \quad \forall \psi \in D(A_i). \quad (1.40)$$

Using the definition of A_i this can be rewritten as

$$(\rho^* \phi, \tilde{A}_i \rho^{-1} \psi) = (\phi, \psi), \quad \forall \psi \in D(A_i). \quad (1.41)$$

Therefore, $\phi \in D(A_i^*) \Leftrightarrow \rho^* \phi \in D(\tilde{A}_i^*) = \theta D(\tilde{A}_i) = \rho^* D(A_i)$, which is equivalent to

$$D(A_i^*) = D(A_i). \quad (1.42)$$

Then, using relations (1.15), it follows from (1.41) that

$$(\phi, \psi) = ((\rho^*)^{-1} \tilde{A}_i^* \rho^* \phi, \psi) = (\rho \tilde{A}_i \rho^{-1} \phi, \psi), \quad \forall \psi \in D(A_i) \quad (1.43)$$

so $A_i = A_i^*$. □

Theorem 1.3 shows that quasi-Hermitian operators can be used as observables in quantum mechanics if we use Hilbert space \mathcal{H}_θ . However, for this to be a viable quantum theory, we must associate the Hilbert space \mathcal{H}_θ with some physical system and then associate the states of this system with vectors in \mathcal{H}_θ .

Let us now suppose that $\mathcal{H} = L^2(\Omega)$, where Ω is some subset of \mathbb{R}^n and let \tilde{H} be a quasi-Hermitian operator, which we want to associate with the Hamiltonian of the system. We choose some metric operator associated with this operator. It is not unique because \tilde{H} is reducible (see Corrolary A.6). Since we know to which system the Hilbert space \mathcal{H} corresponds (one or more spinless particles) and how the functions from this space correspond to the states of this system (using the position and momentum operators (1.5)), we can interpret operator \tilde{H} using Theorem 1.5. We choose some ρ such that $\theta = \rho^* \rho$ and associate the wavefunction $\tilde{\psi} \in \mathcal{H}_\theta$ with the state corresponding to the wavefunction $\psi = \rho \tilde{\psi} \in \mathcal{H}$. In other words as a position resp. momentum operator in \mathcal{H}_θ we choose the operators

$$\hat{x}_i = \rho^{-1} \hat{x}_i \rho, \quad \text{resp.} \quad \hat{p}_i = \rho^{-1} \hat{p}_i \rho. \quad (1.44)$$

These are quasi-Hermitian operators in \mathcal{H} so they are self-adjoint in \mathcal{H}_θ .

Our system is, therefore, described by a set of operators $\tilde{\mathcal{A}} = \{\tilde{H}, \hat{x}_i, \hat{p}_j\}$ on \mathcal{H}_θ . These operators are unitarily equivalent to the operators $\mathcal{A} = \{\rho H \rho^{-1}, \hat{x}_i, \hat{p}_j\}$ on \mathcal{H} . We can, therefore, describe the system either by using the Hilbert space \mathcal{H}_θ , where we don't have standard operators of position and momentum, but instead, presumably more complicated, operators (1.44), or we can use standard Hilbert space $L^2(\Omega)$ with standard operators of position and momentum, but we have to use the operator $\rho H \rho^{-1}$ as a Hamiltonian. Both approaches are equivalent in all physical predictions, including the time evolution (this holds for any unitary transformation).

The decomposition $\theta = \rho^* \rho$ is not unique, different choice of operator ρ leads to a different physical interpretation of quasi-hermitian Hamiltonian \tilde{H} . If we use the Hilbert space \mathcal{H}_θ all such interpretation have the same Hamiltonian, but differ in operators of position and momentum. If we use the Hilbert space \mathcal{H} , the situation is precisely the opposite. All interpretations corresponding to different ρ have the same operators of position and momentum, but they have different Hamiltonians.

We may ask ourselves whether it is possible to interpret \tilde{H} in \mathcal{H}_θ as a Hamiltonian of a system corresponding to $L^2(\Omega)$ in a different way than using some decomposition ρ . Whatever interpretation we choose, we have to define operators of position and momentum (\hat{x}_i, \hat{p}_j) such that they satisfy the canonical commutation relations (CCR)(1.6). We will, for simplicity, restrict ourselves to 1-dimensional case, so that we have only one operator of position and momentum: \hat{x}, \hat{p} .

CCR cannot be satisfied by bounded operators and are, therefore, only formal because of problems with domains. To define them in a proper manner one-parametric unitary groups are

used (see Definition A.1). Let $\tilde{V}(t)$, resp. $\tilde{U}(s)$ be a one-parametric unitary group associated with operator \hat{x} resp. \hat{p} , then, using formal calculations, CCR can be transformed in a relation for associated unitary groups (here we set $\hbar = 1$):

$$\tilde{U}(s)\tilde{V}(t) = e^{ist}\tilde{V}(t)\tilde{U}(s), \quad \forall s, t \in \mathbb{R}. \quad (1.45)$$

These are the so-called Weyl relations. Since $\tilde{V}(t)$, $\tilde{U}(s)$ are bounded operators for any t , s , they are mathematically well defined. Let $V_S(t)$ resp. $U_S(s)$ denote the one-parametric unitary group associated with the operator \hat{x} resp. \hat{p} , this is the so-called Schrödinger representation. As could be expected, it satisfies the Weyl relations. The following theorem shows that up to multiplicity, every solution of Weyl relations is unitarily equivalent to the Schrödinger representation.

Theorem 1.7 (Stone-von Neumann). *Let $V(t), U(s)$ be one-parametric unitary groups on a separable Hilbert space \mathcal{H} satisfying the Weyl relations. Then, there are closed subspaces \mathcal{H}_l such that*

1. $\mathcal{H} = \bigoplus_{l=1}^N \mathcal{H}_l$ (N is a positive integer or ∞)
2. $U(t) : \mathcal{H}_l \rightarrow \mathcal{H}_l, V(s) : \mathcal{H}_l \rightarrow \mathcal{H}_l, \quad \forall s, t \in \mathbb{R}$
3. For each l , there is a unitary operator $T_l : \mathcal{H}_l \rightarrow L^2(\mathbb{R})$ such that $T_l U(t) T_l^{-1} = U_S(t), T_l V(s) T_l^{-1} = V_S(s)$.

The following corollary shows that if one-parametric strongly continuous unitary groups satisfy Weyl relations, then their self-adjoint generators have the desired properties.

Corollary 1.8. *Let $V(t), U(s)$ be one-parametric strongly continuous unitary groups satisfying the Weyl relations and let A, B be their self-adjoint generators, then there exists a dense domain D such that*

1. $A : D \rightarrow D, B : D \rightarrow D$
2. $AB\phi - BA\phi = -i\phi, \quad \forall \phi \in \mathcal{H}$
3. A, B are essentially self-adjoint on \mathcal{H} (this means that their closures are self-adjoint)

See [34, Section VIII.5] for proofs and more informations about this topics. We now suppose that the set $\{\hat{x}, \hat{p}\}$ is irreducible, then also set $\{V(t), U(s) | t, s \in \mathbb{R}\}$ is irreducible. This is so because comutants of both sets are the same and they both satisfy requirements of Schur's lemma. Then according to Theorem 1.7, there exists a unitary operator $\rho : \mathcal{H}_\theta \rightarrow \mathcal{H}$ such that

$$\rho \tilde{V}(t) \rho^{-1} = V_S(t), \quad \rho \tilde{U}(s) \rho^{-1} = U_S(s). \quad (1.46)$$

Using relation (A.7) at $t = 0$, the same also holds for operators $\hat{\hat{x}}, \hat{\hat{p}}$:

$$\rho \hat{\hat{x}} \rho^{-1} = \hat{x}, \quad \rho \hat{\hat{p}} \rho^{-1} = \hat{p}. \quad (1.47)$$

Since ρ is unitary it must hold that

$$(\phi, \psi)_\theta = (\rho\phi, \rho\psi) = (\phi, \rho^* \rho\psi), \quad \phi, \psi \in \mathcal{H} \quad (1.48)$$

and, therefore, $\theta = \rho^* \rho$. The same result also holds in higher dimensions.

We see that if we want to interpret \tilde{H} in \mathcal{H}_θ as a Hamiltonian of a system corresponding to the space $L^2(\Omega)$, then as long as we choose operators of position and momentum irreducibly, the interpretation will be equivalent to choosing some decomposition $\theta = \rho^* \rho$. The ambiguity of this decomposition, therefore, precisely corresponds to different irreducible choices of position and momentum operator. As long as we don't use spin, the condition of irreducibility is natural.

Up to now we have not discussed the ambiguity corresponding to different choices of the metric operator. However, if we choose some position and momentum operators such that they are irreducible in \mathcal{H}_θ , then metric operator is unique because the set $\{\tilde{H}, \hat{\hat{x}}_i, \hat{\hat{p}}_i\}$ is then of course also irreducible.

1.3 \mathcal{PT} -symmetric quantum mechanics

Independently of the theory of quasi-Hermitian operators, there appeared another attempt to use non-self-adjoint operators in quantum mechanics, in the case of the so-called \mathcal{PT} symmetric operators. The interest in these operators was motivated by the discovery by Bender and Boetcher ([8]), that they often have real spectrum despite being non-self-adjoint. In this section, we give a very brief summary of this topic and show its connection to quasi-Hermitian operators. See papers [9] and [7] for overview of \mathcal{PT} -symmetric quantum mechanics or paper [32] for overview of the whole field. For more detailed informations see proceedings of the *International workshops on Pseudo-Hermitian Hamiltonians in Quantum Physics* [27], [28], [29], [18], [30], [2], [1], [35]. Throughout this section we will suppose that our Hilbert space is $L^2(\Omega)$, where Ω is some subset of \mathbb{R}^n , symmetric with respect to 0. Operator \mathcal{PT} is a composition of the operator of spatial inversion \mathcal{P} :

$$\mathcal{P}\psi(x) = \psi(-x) \quad (1.49)$$

and operator of complex conjugation \mathcal{T} :

$$\mathcal{T}\psi = \bar{\psi}. \quad (1.50)$$

\mathcal{T} is an antilinear operator, therefore, also \mathcal{PT} is an antilinear operator. Operator H (possibly non-self-adjoint) is called \mathcal{PT} -symmetric if it commutes with the \mathcal{PT} operator:

$$\mathcal{PT}H\psi = H\mathcal{PT}\psi, \quad \forall \psi \in D(H). \quad (1.51)$$

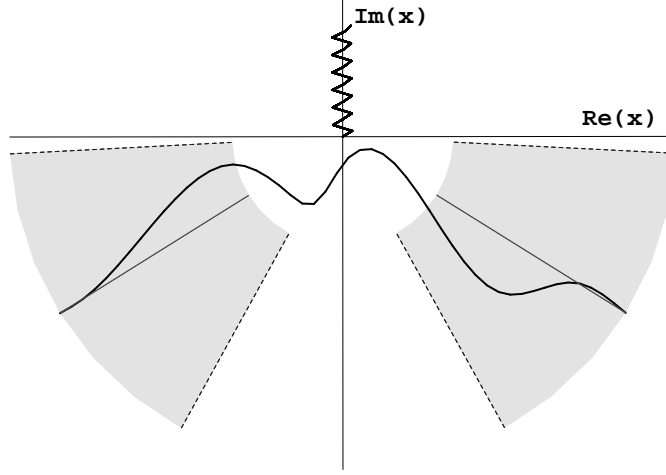


Figure 1: Stoke's wedges for $\epsilon = 2.2$ and a contour lying in these wedges. Source: [7].

If H is a self-adjoint Hamiltonian, \mathcal{PT} symmetry has a direct physical meaning: Hamiltonian is \mathcal{PT} -symmetric if the system is invariant under simultaneous spatial inversion (mirror inversion) and time inversion.

One class of \mathcal{PT} -symmetric Hamiltonians, which was extensively studied is:

$$H_\epsilon = -\frac{d^2}{dx^2} + x^2(ix)^\epsilon, \quad \epsilon \in \mathbb{R}. \quad (1.52)$$

The spectral problem is defined along a contour in a complex plane. The contour must asymptotically lie in the union of the Stoke's wedges (see Fig. 1 for an example of Stoke's wedges):

$$S_\epsilon^\pm = \{r e^{-i(\theta_\epsilon^\pm + \phi)} \mid r \in [0, \infty), \phi \in (-\delta_\epsilon, \delta_\epsilon)\}, \quad (1.53)$$

where

$$\theta_\epsilon^- = -\pi + \frac{\epsilon}{\epsilon + 4} \frac{\pi}{2}, \quad \theta_\epsilon^+ = -\frac{\epsilon}{\epsilon + 4} \frac{\pi}{2}, \quad \delta_\epsilon = \frac{2\pi}{\epsilon + 4}. \quad (1.54)$$

Note that the wedges are \mathcal{PT} symmetric in the sense that

$$S_\epsilon^- = -(S_\epsilon^+)^*. \quad (1.55)$$

If $-1 < \epsilon < 2$ the wedges contain real axis, so we can choose the contour to be real axis. For other values of ϵ the contour must be complex. Fig. 2 shows results of numerical calculation of the spectrum. The spectrum is all real and positive if $\epsilon \geq 0$. If $-1 < \epsilon < 0$, part of the spectrum becomes complex. If $\epsilon \leq -1$ the spectrum is completely complex.

The Hamiltonians (1.52) are \mathcal{P} -self-adjoint, which means that the following relation is satisfied:

$$H^* \mathcal{P} = \mathcal{P} H. \quad (1.56)$$

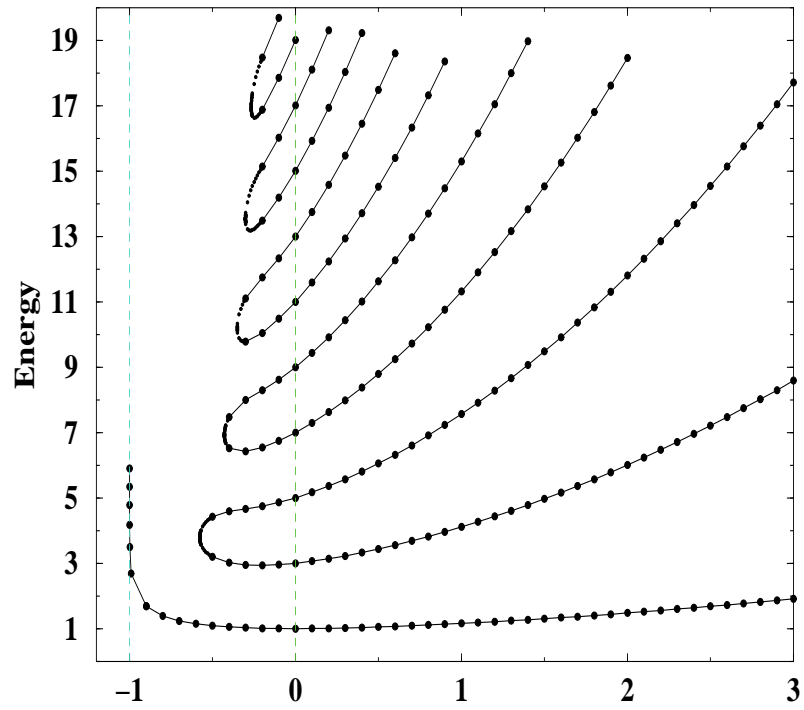


Figure 2: Numerical results of calculation of the spectrum of the Hamiltonians (1.52). Source: [7].

They, therefore satisfy:

$$(H\phi, \psi)_{\mathcal{P}} = (\phi, H\psi)_{\mathcal{P}}, \quad (1.57)$$

where

$$(\phi, \psi)_{\mathcal{P}} = (\phi, \mathcal{P}\psi). \quad (1.58)$$

$(\phi, \psi)_{\mathcal{P}}$ is not a scalar product because it is not positive-definite, this, however, means that H is self-adjoint in Krein space (see Section 1.4).

To interpret Hamiltonians H_{ϵ} as observables in quantum mechanics, using the so-called \mathcal{C} operator was proposed. This is a bounded operator such that:

1. $\mathcal{C}^2 = I$
2. $[\mathcal{C}, H] = 0$
3. $\mathcal{P}\mathcal{C}$ is a positive operator

The \mathcal{C} operator is sometimes called the \mathcal{C} -symmetry operator and if it exists the Hamiltonian is said to possess the \mathcal{C} -symmetry. This is because the \mathcal{C} operator has properties similar to the charge conjugation operator in quantum field theory. If the \mathcal{C} operator exists we can interpret the Hamiltonian in a Hilbert space with scalar product:

$$(\phi, \psi)_{\mathcal{C}} = (\phi, \mathcal{P}\mathcal{C}\psi). \quad (1.59)$$

This is possible because the following theorem holds.

Theorem 1.9. *Let H be a \mathcal{P} -self adjoint operator. If \mathcal{C} operator exists, then H is a quasi-Hermitian operator and $\theta = \mathcal{P}\mathcal{C}$ is a metric operator associated with H .*

Proof. θ is obviously bounded and positive. Its inversion is given by $\theta^{-1} = \mathcal{C}\mathcal{P}$, which is also a bounded operator.. Because \mathcal{C} commutes with H it must hold that $\mathcal{C}D(H) \subset D(H)$. If we multiply this relation by \mathcal{C} , we find that the converse relation also holds, so

$$\mathcal{C}D(H) = D(H). \quad (1.60)$$

Since H is \mathcal{P} -self adjoint, it must hold that

$$D(H^*) = \mathcal{P}D(H). \quad (1.61)$$

Therefore,

$$D(H^*) = \mathcal{P}\mathcal{C}D(H). \quad (1.62)$$

Now it is easy to show that $H^*\mathcal{P}\mathcal{C} = \mathcal{P}\mathcal{C}H$. □

The converse does not hold – if we have quasi-Hermitian operator H with metric θ then in general $\mathcal{P}\theta$ is not a metric operator. The reason is that it will not satisfy the condition $\mathcal{C}^2 = I$.

Remark 1.10. In paper [7], the following was written about \mathcal{PT} -symmetric quantum mechanics:

We emphasize that these new kinds of Hamiltonians define valid and consistent quantum theories in which the mathematical condition of Dirac Hermiticity $H = H^\dagger$ has been replaced by the physical condition of \mathcal{PT} symmetry, $H = H^{\mathcal{PT}}$. The condition [...] that the Hamiltonian is \mathcal{PT} symmetric is a physical condition because \mathcal{P} and \mathcal{T} are elements of the homogeneous Lorentz group of spatial rotations and Lorentz boosts.

This view is problematic for several reasons. Firstly the condition of Hermiticity (called self-adjointness in this work) is not replaced, after all the Hamiltonians are interpreted by finding a scalar product in which they are self-adjoint. Furthermore, the condition of \mathcal{PT} -symmetry is actually not that important in the theory, to interpret the Hamiltonians, crucial ingredient is the \mathcal{C} -operator and \mathcal{PT} -symmetry is neither sufficient nor necessary condition for the existence of the \mathcal{C} operator.

Lastly, in the case of non-self-adjoint operators, \mathcal{PT} -symmetry no longer corresponds to simultaneous mirror and time symmetry because \mathcal{P} no longer corresponds to mirror symmetry. The reason is that if it was a mirror symmetry, then x would have to correspond to position of the particle and then the operator of position would have to be the standard operator of position. Therefore, also the momentum operator would have to be the standard one and they would have to be self-adjoint in the Hilbert space \mathcal{H}_θ , where $\theta = \mathcal{P}\mathcal{C}$. Therefore they would have to commute with the operator $\theta = \mathcal{P}\mathcal{C}$. However, then according to Theorem A.5, $\mathcal{P}\mathcal{C} = cI$ and then H would be self-adjoint. We, therefore, see that \mathcal{P} corresponds to the mirror symmetry, only in the case of self-adjoint operators.

1.4 J -self-adjoint operators in Krein spaces

For mathematical description of non-self-adjoint operators described in previous sections, it can be useful to use Krein spaces. This is so because such operators are often self-adjoint in some Krein space. We first give a short introduction into theory of Krein spaces and then show how they can be used in this context.

1.4.1 Krein spaces

Here we review basic notions from the theory of Krein spaces, for more information see [6]. Let \mathcal{F} be a vector space equipped with an indefinite inner product $[\cdot, \cdot]$. A subspace $V \subset \mathcal{F}$ is

called positive resp. negative if

$$\forall x \in V, x \neq 0, [x, x] > 0 \quad \text{resp.} \quad [x, x] < 0. \quad (1.63)$$

Canonical decomposition is a decomposition:

$$\mathcal{F} = \mathcal{H}_+ \oplus \mathcal{H}_- \quad (1.64)$$

such that \mathcal{H}_+ resp. \mathcal{H}_- is a positive resp. negative subspace satisfying

$$[x_+, x_-] = 0, \quad \forall x_+ \in \mathcal{H}_+, \forall x_- \in \mathcal{H}_-. \quad (1.65)$$

Definition 1.11. \mathcal{F} is called a **Krein space** if it admits a canonical decomposition such that \mathcal{H}_+ resp. \mathcal{H}_- is a Hilbert space with respect to the norm $\sqrt{[x, x]}$ resp. $\sqrt{-[x, x]}$.

Krein space is also a Hilbert space because decomposition (1.64) defines a (positive definite) scalar product

$$(x, y) = [x_+, y_+] - [x_-, y_-], \quad (1.66)$$

$$x = x_+ + x_-, \quad x_+ \in \mathcal{H}_+, x_- \in \mathcal{H}_-, \quad (1.67)$$

$$y = y_+ + y_-, \quad y_+ \in \mathcal{H}_+, y_- \in \mathcal{H}_-. \quad (1.68)$$

We will denote this Hilbert space by \mathcal{H} . Let P_+ resp. P_- denote the orthogonal projection (with respect to scalar product (1.66)) on the subspace \mathcal{H}_+ resp. \mathcal{H}_- and let $J := P_+ - P_-$. This operator is called the **canonical symmetry** of the Krein space \mathcal{F} . This operator relates the scalar product and the indefinite inner product:

$$[x, y] = (x, Jy), \quad (x, y) = [x, Jy]. \quad (1.69)$$

It has the following properties:

$$J^2 = I, \quad (1.70)$$

$$J^* = J. \quad (1.71)$$

Adjoint of a densely defined operator A in Krein space (J -adjoint) is defined by:

$$D(A^{[*]}) = \{x \in \mathcal{F} \mid \exists z \in \mathcal{F}; [x, Ay] = [z, y]; \forall y \in D(A)\}, \quad (1.72)$$

$$A^{[*]}x = z. \quad (1.73)$$

A is called self-adjoint in Krein space (J -self-adjoint) if $A^{[*]} = A$. Obviously, self-adjoint operators are operators that satisfy:

$$A^*J = JA, \quad (1.74)$$

where A^* denotes the adjoint of A in \mathcal{H} . Let \mathcal{H} be a Hilbert space, then any operator J satisfying (1.70), (1.71) defines a Krein space through relations (1.69) and:

$$\mathcal{H}_+ = \frac{1}{2}(I + J)\mathcal{H}, \quad (1.75)$$

$$\mathcal{H}_- = \frac{1}{2}(I - J)\mathcal{H}. \quad (1.76)$$

1.4.2 Connection to \mathcal{PT} -symmetry

The operator \mathcal{P} obviously satisfies conditions: (1.70), (1.71), so it defines a Krein space with indefinite metric:

$$[\phi, \psi] = (\phi, P\psi). \quad (1.77)$$

The reason why Krein space formalism is relevant is that \mathcal{PT} -symmetric Hamiltonians are typically also \mathcal{P} -self-adjoint so they are self-adjoint in this Krein space. This property is not as strong as self-adjointness in the Hilbert space, for example, it does not guarantee the reality of the spectrum, but it can still be useful. For instance, in paper [26] Krein space formalism was used to find the conditions for reality of the spectrum of \mathcal{P} -self-adjoint perturbations of self-adjoint operators. This is one of their results:

Theorem 1.12. *Let A_ϵ , $0 \leq \epsilon \leq 1$, be a family of self-adjoint operators in a Krein space K such that for one (and hence for all) $z \in \rho(A_\epsilon)$ the resolvents $(A_\epsilon - z)^{-1}$ depend continuously on ϵ in the uniform operator topology for $0 \leq \epsilon \leq 1$. Let λ_0 be an isolated real eigenvalue of A_0 with a one-dimensional algebraic eigenspace. Denote by $\lambda(\epsilon)$, $0 \leq \epsilon \leq 1$, the corresponding eigenvalue of A_ϵ which depends continuously on ϵ and is such that $\lambda(0) = \lambda_0$. If for $0 \leq \epsilon \leq \epsilon_0$ the eigenvalue $\lambda(\epsilon)$ did not meet any other eigenvalue of A_ϵ , then $\lambda(\epsilon)$ is real and algebraically simple for all $0 \leq \epsilon \leq \epsilon_0$.*

Krein spaces also allow an elegant way of describing the \mathcal{C} -operator. We define \mathcal{C} -operator for any J -self adjoint operator.

Definition 1.13. Let A be a J -self adjoint operator. It has the property of \mathcal{C} -symmetry if there exists a bounded linear operator \mathcal{C} such that

1. $\mathcal{C}^2 = I$
2. $AC = CA$
3. $J\mathcal{C} > 0$

The following proposition connects the existence of the \mathcal{C} -operator to the existence of a different decomposition of the form (1.64). See [25] for proof.

Proposition 1.14. *Let A be a J -self-adjoint operator. Then A has the property of C -symmetry if and only if A admits the decomposition*

$$A = A_+ \oplus A_-, \quad A_+ = A|_{\mathcal{L}_+}, \quad A_- = A|_{\mathcal{L}_-} \quad (1.78)$$

with respect to a certain choice of decomposition of the type (1.64). The \mathcal{C} operator is given by $\mathcal{C} = P_{\mathcal{L}_+} - P_{\mathcal{L}_-}$, where $P_{\mathcal{L}_\pm}$ are orthogonal projections on subspaces \mathcal{L}_\pm .

For other examples showing how can the Krein spaces be used in this context, see [5], [4] and references therein.

2 The model

In this section we present a simple \mathcal{PT} -symmetric model, originally defined in [21]. The Hamiltonian of the model is a free particle Hamiltonian with complex boundary conditions defined on the Hilbert space $\mathcal{H} = L^2((-a, a))$:

$$H_\alpha \psi = -\psi'', \quad (2.1)$$

$$D(H_\alpha) = \{\psi \in W^{2,2}((-a, a)) | \psi'(-a) + i\alpha\psi(-a) = \psi'(a) + i\alpha\psi(a) = 0\}, \quad (2.2)$$

where α is any real number. For $\alpha \neq 0$ it is not self-adjoint, in fact it satisfies:

$$H_\alpha^* = H_{-\alpha}, \quad (2.3)$$

but it is \mathcal{P} -self-adjoint so it is self-adjoint in a Krein space with inner product $[\phi, \psi] = (\phi, \mathcal{P}\psi)$, where (\cdot, \cdot) is a scalar product in \mathcal{H} . It is also \mathcal{T} -self-adjoint, meaning again that

$$H_\alpha^* \mathcal{T} = \mathcal{T} H_\alpha^*. \quad (2.4)$$

This is a different property than \mathcal{P} -self-adjointness because \mathcal{T} is an antilinear operator. H_α is m -sectorial and it is, therefore, closed, so the spectral problem is well-defined.

This model together with [39] is in a way the simplest \mathcal{PT} -symmetric model possible because its non-Hermiticity is caused solely by the boundary condition. For higher-dimensional generalizations of the model we refer to [15], [14], [23] and [22].

The spectrum of H_α and H_α^* is real and positive, it is given by:

$$\sigma(H_\alpha) = \sigma(H_\alpha^*) = \{\alpha^2\} \cup \{k_j^2\}_{j=1}^\infty, \text{ where } k_j = \frac{j\pi}{2a}, \quad (2.5)$$

The plot of the spectrum is on Fig. 3. The eigenfunctions of H_α resp. H_α^* are

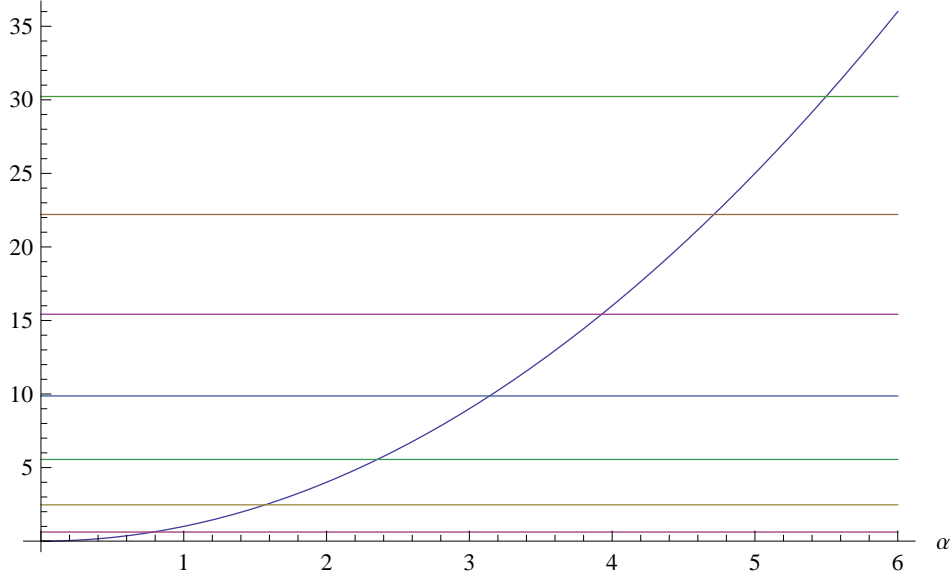


Figure 3: The plot of the spectrum of H_α for $a = 2$.

$$\psi_j^\alpha = \begin{cases} A_0^\alpha e^{-i\alpha(x+a)} & \text{if } j = 0, \\ A_j^\alpha \left(\cos(k_j(x+a)) - i \frac{\alpha}{k_j} \sin(k_j(x+a)) \right) & \text{if } j \geq 1, \end{cases}$$

resp. (2.6)

$$\phi_j^\alpha = \begin{cases} \frac{1}{\sqrt{2a}} e^{i\alpha(x+a)} & \text{if } j = 0, \\ \frac{1}{\sqrt{a}} \left(\cos(k_j(x+a)) + i \frac{\alpha}{k_j} \sin(k_j(x+a)) \right) & \text{if } j \geq 1, \end{cases}$$

If the following condition is satisfied

$$\alpha \neq \frac{j\pi}{2a}, \quad \forall j \in \mathbb{Z}, \quad (2.7)$$

and if we choose the normalization constants A_j^α according to the equations:

$$1 = A_0^\alpha \frac{1}{\sqrt{2a}} \frac{1 - e^{-4i\alpha a}}{2i\alpha}, \quad (2.8)$$

$$1 = A_j^\alpha \sqrt{a} \frac{(k_j^2 - \alpha^2)}{k_j^2} \quad j \geq 1, \quad (2.9)$$

then functions $\{\psi_j^\alpha, \phi_k^\alpha\}$ form a biorthonormal basis, i.e.

$$(\phi_j^\alpha, \psi_k^\alpha) = \delta_{jk}, \quad \forall j, k \geq 0, \quad (2.10)$$

$$\psi = \sum_{j=0}^{\infty} \psi_j^\alpha (\phi_j^\alpha, \psi) = \sum_{j=0}^{\infty} \phi_j^\alpha (\psi_j^\alpha, \psi), \quad \forall \psi \in \mathcal{H}. \quad (2.11)$$

Remark 2.1. In paper [21] the interval $(0, d)$ was used instead of interval $(-a, a)$ which we use here. This is just a formal difference because when we set $d = 2a$, then Hamiltonian (2.2)

and Hamiltonian defined on the interval $(0, d)$ are connected by unitary transformation U :

$$(U\psi)(x) = \psi(x - a). \quad (2.12)$$

3 Metric operator

It was demonstrated in [21] that the series

$$\eta_\alpha = \sum_{n=0}^{\infty} \phi_n^\alpha(\phi_n^\alpha, \cdot) \quad (3.1)$$

strongly converges to a metric operator provided that the condition (2.7) is satisfied. In the following we will always understand series of this type in the strong sense. General metric operator can be expressed in a similar form:

Theorem 3.1. *Let $\alpha \in \mathbb{R} \setminus \{\frac{j\pi}{2a}\}_{j=-\infty}^{\infty}$ and let $\{c_n^\alpha\}$ be a sequence of real numbers such that*

$$\exists m^\alpha, M^\alpha > 0, \quad m^\alpha < c_n^\alpha < M^\alpha, \quad \forall n \in \mathbb{N}, \quad (3.2)$$

Then the series

$$\theta_\alpha = \sum_{n=0}^{\infty} c_n^\alpha \phi_n^\alpha(\phi_n^\alpha, \cdot) \quad (3.3)$$

strongly converges to a metric operator associated with the Hamiltonian H_α . Conversely, all metric operators of H_α can be expressed in the form (3.3).

Proof. a) We first prove that the series (3.3) is a metric operator. We denote

$$\rho = \sqrt{\eta_\alpha}. \quad (3.4)$$

Since the operator $H_\alpha^F = \rho H_\alpha \rho^{-1}$ is a self-adjoint operator with pure discrete spectrum, its eigenfunctions, given by:

$$e_n^\alpha = \rho \psi_n^\alpha = \rho^{-1} \phi_n^\alpha \quad (3.5)$$

form an orthonormal basis (note that $\eta_\alpha \psi_n^\alpha = \phi_n^\alpha$). The series (3.3) strongly converges because for any $\psi \in \mathcal{H}$

$$\theta_\alpha = \sum_{n=0}^{\infty} c_n^\alpha \phi_n^\alpha(\phi_n^\alpha, \psi) = \rho \left(\sum_{n=0}^{\infty} c_n^\alpha e_n^\alpha(e_n^\alpha, \psi) \right) \rho \quad (3.6)$$

and series $\sum_{n=0}^{\infty} e_k(e_k, \psi)$ is convergent. It follows that θ_α is a bounded operator because it is a composition of bounded operators. Similarly we can show that the series

$$M = \sum_{n=0}^{\infty} \frac{1}{c_n} \phi_n^\alpha(\phi_n^\alpha, \cdot) \quad (3.7)$$

strongly converges to a bounded operator and since $M\theta_\alpha = I$, M must be the inversion of θ_α . θ_α is a positive operator because, using the biorthonormality of $\{\psi_k, \phi_k\}$ and expanding ψ into the biorthonormal basis (2.11): ,

$$(\psi, \theta_\alpha \psi) = \sum_{k=0}^{\infty} \sum_{n=0}^{\infty} \overline{(\phi_k^\alpha, \psi)} (\phi_n^\alpha, \psi) (\psi_k, \theta \psi_n) = \sum_{k=0}^{\infty} c_k |(\phi_k^\alpha, \psi)|^2 > 0, \quad (3.8)$$

where we have used

$$\theta_\alpha \psi_n^\alpha = c_n^\alpha \phi_n^\alpha. \quad (3.9)$$

We now have to show that θ_α satisfies the relation (1.15). It is useful to write this relation for the resolvents instead

$$(H_\alpha^* - \lambda)^{-1} = (\theta H_\alpha \theta^{-1} - \lambda)^{-1} = \theta (H_\alpha - \lambda)^{-1} \theta^{-1}, \quad (3.10)$$

where λ is any number not in the spectrum of H_α . Therefore, relation (1.15) is equivalent to relation:

$$(H_\alpha^* - \lambda)^{-1} \theta = \theta (H_\alpha - \lambda)^{-1}. \quad (3.11)$$

Let $\psi \in \mathcal{H}$, then using the decomposition (2.11):

$$(H_\alpha^* - \lambda)^{-1} \theta \psi = (H_\alpha^* - \lambda)^{-1} \theta \sum_{j=0}^{\infty} \psi_j^\alpha (\phi_j^\alpha, \psi) \quad (3.12)$$

$$= (H_\alpha^* - \lambda)^{-1} \sum_{j=0}^{\infty} c_j \phi_j^\alpha (\phi_j^\alpha, \psi) = \sum_{j=0}^{\infty} \frac{c_j}{\lambda_n - \lambda} \phi_j^\alpha (\phi_j^\alpha, \psi), \quad (3.13)$$

where λ_n is the eigenvalue of H_α corresponding to ψ_k^α . Similarly

$$\theta (H_\alpha - \lambda)^{-1} \psi = \theta \sum_{j=0}^{\infty} \frac{1}{\lambda_n - \lambda} \psi_j^\alpha (\phi_j^\alpha, \psi) = \sum_{j=0}^{\infty} \frac{c_j}{\lambda_n - \lambda} \phi_j^\alpha (\phi_j^\alpha, \psi). \quad (3.14)$$

θ_α is, therefore, a metric operator.

b) We now prove that every metric operator θ_α has the form (3.3) with sequence $\{c_n^\alpha\}$ satisfying (3.2). From the condition (1.15) we find that

$$H_\alpha^* \theta_\alpha \phi_n^\alpha = \theta_\alpha H_\alpha \psi_n^\alpha = \lambda_n^\alpha \theta_\alpha \psi_n^\alpha, \quad (3.15)$$

$\theta_\alpha \psi_k^\alpha$ is, therefore, an eigenfunction of H_α^* and since its spectrum is not degenerate it must be a multiple of ϕ_k^α :

$$\theta_\alpha \psi_n^\alpha = c_n^\alpha \phi_n^\alpha. \quad (3.16)$$

Using the decomposition into the birthnormal basis (2.11)

$$\theta_\alpha \psi = \sum_{n=0}^{\infty} c_n \phi_n^\alpha(\phi_n^\alpha, \psi). \quad (3.17)$$

Numbers c_k must be positive because θ_α is a positive operator:

$$0 < (\psi_n^\alpha, \theta_\alpha \psi_n^\alpha) = c_n^\alpha. \quad (3.18)$$

Boundedness of sequence $\{c_n\}$ follows from relation (3.6) because if it was not bounded, then operator $\sum_{n=0}^{\infty} c_n e_n(e_n, \psi)$ would not be bounded and, therefore, neither would be operator θ_α . Similarly, by again using the decomposition into the birthnormal basis (2.11) we can show that the inversion of θ_α has the form (3.7) and since it is bounded, the sequence $\{\frac{1}{c_n}\}$ must also be bounded. \square

Remark 3.2. Note, that this result has already been partly proven in [38]. There it was shown that a metric operator θ of an operator A with purely discrete spectrum has the form

$$\theta = \sum_{n=0}^{\infty} \phi_n(\phi_n, \cdot), \quad (3.19)$$

where ϕ_j are eigenfunctions of A^* , if eigenfunctions of A (denoted by ψ_j) and A^* are normalized in a special way, namely:

$$(\phi_j, \psi_k) = \delta_{jk}, \quad \theta \psi_n = \phi_n. \quad (3.20)$$

Expression (3.3) can be derived from this result by renormalizing functions $\phi_j^\alpha, \psi_j^\alpha$

$$\tilde{\phi}_n^\alpha = \sqrt{c_n} \phi_n^\alpha \quad \tilde{\psi}_n^\alpha = \frac{1}{\sqrt{c_n}} \psi_n^\alpha \quad (3.21)$$

because these functions satisfy normalization (3.20).

The series (3.1) was summed up in paper [20] using the functional calculus. This approach cannot be used for general values of $\{c_n\}$, but it can be used to simplify the series (3.3) considerably. Indeed now we show how to transform the problem of finding a metric operator associated with the operator H_α to the problem of finding a metric operator associated with the Neumann Laplacian. This significantly simplifies the problem, since Neumann Laplacian is self-adjoint and its metric operators are, therefore, operators with which it commutes and which are positive, bounded and have bounded inversion. Our results are summarized in the following theorem.

Theorem 3.3. *Let θ_α be a linear operator on the Hilbert space \mathcal{H} , then it is a metric operator associated with the Hamiltonian (2.2) if and only if there exists metric operator J_N^α associated with the Neumann Laplacian, such that*

$$\theta_\alpha = c_0^\alpha T_1^\alpha + J_N^\alpha (I + T_2^\alpha) - i \frac{d}{dx} J_N^\alpha T_3^\alpha, \quad (3.22)$$

where c_0^α is a number given by $\frac{1}{\chi_0^N} J_N^\alpha \chi_0^N$ and T_1^α , T_2^α , T_3^α are integral operators with the following kernels:

$$\mathcal{T}_1^\alpha(x, y) = \frac{1}{2a} \left(e^{i\alpha(y-x)} - 1 \right), \quad (3.23)$$

$$\mathcal{T}_2^\alpha(x, y) = \frac{i\alpha}{2a} y + \frac{i\alpha}{2} \operatorname{sgn}(x - y), \quad (3.24)$$

$$\begin{aligned} \mathcal{T}_3^\alpha(x, y) = & \frac{\alpha}{12a} \left(y^2(3 - i\alpha y) + 3x^2(1 - i\alpha y) + 2a^2(1 + i\alpha(3x + y)) \right) \\ & - \frac{1}{4} i\alpha \left(-2i + \alpha(x - y) \right) (x - y) \operatorname{sgn}(x - y). \end{aligned} \quad (3.25)$$

Proof. To prove the theorem we show that series (3.3) can be written in desired form. Functions ϕ_j^α for $j > 1$ can be written as

$$\phi_j^\alpha = \chi_j^N + \frac{i\alpha}{k_j} \chi_j^D, \quad (3.26)$$

where χ_j^N resp. χ_j^D are eigenfunctions of the Neumann resp. Dirichlet Laplacian (see Appendix A). Thus series (3.3) can be decomposed as

$$\begin{aligned} \theta_\alpha = & c_0^\alpha \phi_0^\alpha(\phi_0^\alpha, \cdot) - c_0^\alpha \chi_0^N(\chi_0^N, \cdot) + \sum_{n=0}^{\infty} c_n^\alpha \chi_n^N(\chi_n^N, \cdot) \\ & + \alpha^2 \sum_{n=1}^{\infty} \frac{c_n^\alpha}{k_n^2} \chi_n^D(\chi_n^D, \cdot) + i\alpha \sum_{n=1}^{\infty} \frac{c_n^\alpha}{k_n} \chi_n^D(\chi_n^N, \cdot) - i\alpha \sum_{n=1}^{\infty} \frac{c_n^\alpha}{k_n} \chi_n^N(\chi_n^D, \cdot). \end{aligned} \quad (3.27)$$

We now introduce the operators:

$$J_N^\alpha = \sum_{n=0}^{\infty} c_n^\alpha \chi_n^N(\chi_n^N, \cdot), \quad (3.28)$$

$$J_D^\alpha = \sum_{n=1}^{\infty} c_n^\alpha \chi_n^D(\chi_n^D, \cdot). \quad (3.29)$$

These are bounded self-adjoint operators, satisfying $J_N^\alpha \chi_n^N = c_n^\alpha \chi_n^N$ resp. $J_D^\alpha \chi_n^D = c_n^\alpha \chi_n^D$. Using these operators, expression (3.27) can be rewritten as

$$\begin{aligned} \theta_\alpha = & c_0^\alpha \phi_0^\alpha(\phi_0^\alpha, \cdot) - c_0^\alpha \chi_0^N(\chi_0^N, \cdot) + J_N^\alpha \left(\sum_{n=0}^{\infty} \chi_n^N(\chi_n^N, \cdot) - i\alpha \sum_{n=1}^{\infty} \frac{1}{k_n} \chi_n^N(\chi_n^D, \cdot) \right) \\ & + J_D^\alpha \left(\alpha^2 \sum_{n=1}^{\infty} \frac{1}{k_n^2} \chi_n^D(\chi_n^D, \cdot) + i\alpha \sum_{n=1}^{\infty} \frac{1}{k_n} \chi_n^D(\chi_n^N, \cdot) \right). \end{aligned} \quad (3.30)$$

Dependence of θ_α on the sequence $\{c_n^\alpha\}$ is now contained in the operators J_N^α and J_D^α . The part not depending on $\{c_n^\alpha\}$ can be summed up using the spectral theorem in the same way as in [20]. We first define a ‘‘momentum’’ operator p :

$$\begin{aligned} p\psi &= -i\psi', \\ D(p) &= \{\varphi \in W^{1,2}((-a, a)) \mid \varphi(-a) = \varphi(a) = 0\}. \end{aligned} \quad (3.31)$$

The adjoint of p acts in the same way, but has domain $D(p^*) = W^{1,2}((-a, a))$. p fulfills the following relations

$$p\chi_j^D = -ik_j\chi_j^N, \quad p^*\chi_j^N = ik_j\chi_j^D. \quad (3.32)$$

We can now modify (3.30) so that it no longer contains series with both χ_j^N and χ_j^D :

$$\begin{aligned} \theta_\alpha &= c_0^\alpha \phi_0^\alpha(\phi_0^\alpha, \cdot) - c_0^\alpha \chi_0^N(\chi_0^N, \cdot) + J_N^\alpha \left(\sum_{n=0}^{\infty} \chi_n^N(\chi_n^N, \cdot) + \alpha p \sum_{n=1}^{\infty} \frac{1}{k_n^2} \chi_n^D(\chi_n^D, \cdot) \right) \\ &\quad + J_D^\alpha \left(\alpha^2 \sum_{n=1}^{\infty} \frac{1}{k_n^2} \chi_n^D(\chi_n^D, \cdot) + \alpha p^* \sum_{n=1}^{\infty} \frac{1}{k_n^2} \chi_n^N(\chi_n^N, \cdot) \right). \end{aligned} \quad (3.33)$$

The Dirichlet and Neumann Laplacians (denoted by $-\Delta_N$ resp. $-\Delta_D$) are self-adjoint operators with compact resolvents and their spectrum is $\{k_j^2\}_{j=1}^{\infty}$ resp. $\{k_j^2\}_{j=0}^{\infty}$ for Neumann Laplacian. It follows from the functional calculus that

$$\sum_{n=0}^{\infty} \chi_n^N(\chi_n^N, \cdot) = I, \quad (3.34)$$

$$\sum_{n=1}^{\infty} \frac{1}{k_n^2} \chi_n^D(\chi_n^D, \cdot) = (-\Delta_D)^{-1}, \quad (3.35)$$

$$\sum_{n=1}^{\infty} \frac{1}{k_n^2} \chi_n^N(\chi_n^N, \cdot) = (-\Delta_N^\perp)^{-1}, \quad (3.36)$$

where $(-\Delta_N^\perp)^{-1}$ is the reduced resolvent of the Neumann Laplacian with respect to the 0 eigenvalue (see [19, section III-§6.5] for the definition of the reduced resolvent). We, therefore, have the following expression for the metric operator:

$$\begin{aligned} \theta_\alpha &= c_0^\alpha \phi_0^\alpha(\phi_0^\alpha, \cdot) - c_0^\alpha \chi_0^N(\chi_0^N, \cdot) + J_N^\alpha (I + \alpha p(-\Delta_D)^{-1}) \\ &\quad + J_D^\alpha \left(\alpha^2 (-\Delta_D)^{-1} + i\alpha (-\Delta_N^\perp)^{-1} \right). \end{aligned} \quad (3.37)$$

The series J_D^α can be expressed using the series J_N^α as

$$J_D^\alpha = p^* J_N^\alpha p (-\Delta_D)^{-1}. \quad (3.38)$$

Indeed:

$$\begin{aligned} p^* J_N^\alpha p (-\Delta_D)^{-1} &= p^* J_N^\alpha p \sum_{n=1}^{\infty} \frac{1}{k_n^2} \chi_n^D(\chi_n^D, \cdot) = p^* J_N^\alpha \sum_{n=1}^{\infty} \frac{-i}{k_n} \chi_n^N(\chi_n^D, \cdot) \\ &= p^* \sum_{n=1}^{\infty} c_n^\alpha \frac{-i}{k_n} \chi_n^N(\chi_n^D, \cdot) = \sum_{n=1}^{\infty} c_n^\alpha \chi_n^D(\chi_n^D, \cdot) = J_D^\alpha. \end{aligned} \quad (3.39)$$

Expression (3.37) can thus be rewritten as:

$$\begin{aligned}\theta_\alpha &= c_0^\alpha \phi_0^\alpha(\phi_0^\alpha, \cdot) - c_0^\alpha \chi_0^N(\chi_0^N, \cdot) + J_N^\alpha (I + \alpha p(-\Delta_D)^{-1}) \\ &\quad + p^* J_N^\alpha p(-\Delta_D)^{-1} \left(\alpha^2 (-\Delta_D)^{-1} + i\alpha (-\Delta_N^\perp)^{-1} \right).\end{aligned}\quad (3.40)$$

Now we have to show that J_N^α is indeed a metric operator associated with the Neumann Laplacian and that every such metric operator can be expressed in the form (3.28). This is a statement very similar to Theorem 3.1 and can be proven analogously. The only difference is that one has to consider $\rho = I$ and use the orthonormal basis χ_n^N instead of biorthonormal basis.

It remains to prove that operators T_1^α , T_2^α and T_3^α are integral operators with kernels (3.23)-(3.25). It is a well known fact, that $(-\Delta_D)^{-1}$ is an integral operator, its kernel is a Green's function of differential equation $-\psi'' = f$ with Dirichlet boundary conditions (see e.g. [16, section II-§6] for more details):

$$K_D(x, y) = \frac{(x+a)(a-y)}{2a} \vartheta(y-x) + \frac{(y+a)(a-x)}{2a} \vartheta(x-y), \quad (3.41)$$

where ϑ is the Heaviside step function. We can now calculate the operator $p(-\Delta_D)^{-1}$ using the following lemma

Lemma 3.4. *Let $f_1, f_2 \in C^1(-a, a)$, $g_1, g_2 \in L^2(-a, a)$ and*

$$\mathcal{K}(x, y) = f_1(x)g_1(y)\vartheta(x-y) + f_2(x)g_2(y)\vartheta(y-x), \quad (3.42)$$

Then for any $\psi \in L^2(-a, a)$:

$$\begin{aligned}\frac{d}{dx} \int_{-a}^a \mathcal{K}(x, y)\psi(y)dy &= \int_{-a}^a \left(f_1'(x)g_1(y)\vartheta(x-y) + f_2'(x)g_2(y)\vartheta(y-x) \right) \psi(y)dy \\ &\quad + f_1(x)g_1(x)\psi(x) - f_2(x)g_2(x)\psi(x).\end{aligned}\quad (3.43)$$

Remark 3.5. This lemma means that when differentiating the expression $\int_{-a}^a \mathcal{K}(x, y)\phi(y)dy$, we can formally differentiate the kernel \mathcal{K} as a distribution.

Proof. Proof immediately follows by differentiating

$$\mathcal{K}(x, y)\psi(y)dy = f_1(x) \int_{-a}^x g_1(y)\psi(y)dy + f_2(x) \int_x^a g_2(y)\psi(y)dy. \quad (3.44)$$

□

$p(-\Delta_D)^{-1}$ is, therefore, also an integral operator with kernel:

$$K_D^P(x, y) = \frac{i}{2a}y + \frac{i}{2}\text{sgn}(x-y). \quad (3.45)$$

$p^*(-\Delta_N^\perp)^{-1}$ is also an integral operator with kernel:

$$K_N(x, y) = -\frac{i}{2a}x + \frac{i}{2}\text{sgn}(x - y). \quad (3.46)$$

To see this, we first note that $(-\Delta_N^\perp)^{-1}$ is an inversion of the Neumann Laplacian in the following sense:

$$(-\Delta_N^\perp)^{-1} = (-\Delta_N|_{\{\chi_0^N\}^\perp})^{-1}P, \quad (3.47)$$

where P is an orthogonal projector on subspace orthogonal to χ_0^N . This means that $(-\Delta_N^\perp)^{-1}f$ for $f \perp \chi_0^N$ gives the solution of differential equation $-\Delta_N\psi = f$, which is orthogonal to χ_0^N . It is an integral operator and its kernel is the so-called modified Green's function of equation $-\Delta_N\psi = f$ (see [40, section 5.2] for more details). It is given by

$$G_N(x, y) = \frac{x^2 + y^2}{4a} + \frac{x + y}{2} + \frac{a}{6} - y\vartheta(y - x) - x\vartheta(x - y). \quad (3.48)$$

Formula (3.46) then again follows by Lemma 3.4. To finish the proof, one only has to compose the operator $p(-\Delta_D)^{-1}$ with operator $\alpha^2(-\Delta_D)^{-1} + i\alpha(-\Delta_N^\perp)^{-1}$, which yields the operator T_3^α . \square

From the proof it immediately follows another useful expression for the metric operator:

Theorem 3.6. *Let θ_α be a linear operator in the Hilbert space \mathcal{H} , then it is a metric operator associated with the Hamiltonian H_α if and only if there exists a sequence $\{c_n^\alpha\}$ satisfying (3.2) such that*

$$\theta_\alpha = c_0^\alpha T_1^\alpha + J_N^\alpha(I + T_2^\alpha) + J_D^\alpha T_4^\alpha, \quad (3.49)$$

where J_N^α and J_D^α are operators (3.28) resp. (3.29) and T_4^α is an integral operator with kernel:

$$\mathcal{T}_4^\alpha(x, y) = \frac{\alpha^2 a}{2} - \frac{\alpha^2}{2a}xy - \frac{i\alpha}{2a}x + \left(\frac{i\alpha}{2} - \frac{\alpha^2}{2}(x - y)\right)\text{sgn}(x - y). \quad (3.50)$$

Proof. Proof follows from the equation (3.37) and from the integral kernels (3.41)-(3.46). \square

3.1 Dense subset of metric operators

Theorem 3.3 can be used to explicitly construct many different metric operators. In this section we prove that such operators form a dense subset of all metric operators in the strong topology, or in other words we show that for any metric operator θ , there exists a sequence of metrical operators θ_k , which can be found explicitly, such that θ_k strongly converges to θ .

For some sequence $\{c_n\}$ we can use Theorem 3.3 to find the corresponding metric operator if we can sum up the series

$$J_N^\alpha = \sum_{n=0}^{\infty} c_n^\alpha \chi_n^N(\chi_n^N, \cdot). \quad (3.51)$$

Using functional calculus

$$J_N^\alpha = f(-\Delta_N), \quad (3.52)$$

where f is any Borel function satisfying

$$f(k_n^2) = c_n^\alpha. \quad (3.53)$$

This could be calculated explicitly if f was a polynomial, but that cannot happen because then the operator J_N^α would not be bounded. For this reason it is better to write J_N^α (without the term $c_0^\alpha \chi_0^N(\chi_0^N, \cdot)$) as a function of operator

$$I + \lambda(-\Delta_D - \lambda)^{-1} = (-\Delta_N)(-\Delta_N - \lambda)^{-1} = \sum_{n=1}^{\infty} \frac{k_n^2}{k_n^2 - \lambda} \chi_n^N(\chi_n^N, \cdot), \quad (3.54)$$

where λ is a real number smaller than $\frac{\pi^2}{4a^2}$ (so that it is a positive operator). It is more convenient to use Theorem 3.6 instead Theorem 3.3. Operator J_D^α can be expressed as a function of

$$I + \lambda(-\Delta_D - \lambda)^{-1} = \sum_{n=1}^{\infty} \frac{k_n^2}{k_n^2 - \lambda} \chi_n^D(\chi_n^D, \cdot). \quad (3.55)$$

If q is a polynomial such that

$$\exists m > 0, \quad q\left(\frac{k_n^2}{k_n^2 - \lambda}\right) > m, \quad \forall n \geq 1, \quad (3.56)$$

then the operator

$$\theta = c_0 T_1 + J_p^N(I + T_2) + J_p^D T_4, \quad (3.57)$$

where

$$J_q^N = c_0 \chi_0^N(\chi_0^N, \cdot) + q(I + \lambda(-\Delta_N - \lambda)^{-1}), \quad J_q^D = q(I + \lambda(-\Delta_D - \lambda)^{-1}) \quad (3.58)$$

is a metric operator. The resolvents of the Neumann resp. Dirichlet Laplacian are integral operators with explicit and simple kernels, therefore, also operators J_q^N , J_q^D can be found explicitly and they can be expressed as a sum of integral operator and identity operator. The following proposition shows that any operators J^N and J^D can be approximated by such operators J_p^N and J_p^D .

Proposition 3.7. *Let J^N and J^D be operators (3.28) resp. (3.29). Then there exists a sequence of operators $J_{p_k}^N$, $J_{p_k}^D$*

$$J_{p_k}^N = \sum_{n=0}^{\infty} \tilde{c}_n^k \chi_n^N(\chi_n^N, \cdot), \quad J_{p_k}^D = \sum_{n=1}^{\infty} \tilde{c}_n^k \chi_n^D(\chi_n^D, \cdot) \quad (3.59)$$

with $\{\tilde{c}_n^k\}$ satisfying (3.2) and

$$\tilde{c}_n^k = q_k(c_n), \quad n \geq 1, \quad (3.60)$$

for some sequence of polynomials q_k , such that

$$J^N = s\text{-}\lim_{k \rightarrow \infty} J_{q_k}^N, \quad (3.61)$$

$$J^D = s\text{-}\lim_{k \rightarrow \infty} J_{q_k}^D. \quad (3.62)$$

Proof. We denote

$$\lambda_n = \frac{k_n^2}{k_n^2 - \lambda}, \quad \tilde{J}^N = \sum_{n=1}^{\infty} c_n \chi_n^N(\chi_n^N, \cdot), \quad (3.63)$$

$$A_D = I + \lambda(-\Delta_D - \lambda)^{-1}, \quad A_N = I + \lambda(-\Delta_N - \lambda)^{-1}. \quad (3.64)$$

Obviously $\lambda_n \in [1, \lambda_1]$. For every $k \in \mathbb{N}$, there exists a continuous function $f_k : [1, \lambda_1] \rightarrow \mathbb{R}$ such that

$$f_k(\lambda_n) = c_n, \quad \forall n < k, \quad (3.65)$$

$$m < f_k(x) < M, \quad \forall x \in \mathbb{R}. \quad (3.66)$$

For any $\psi \in \mathcal{H}$

$$\|(\tilde{J}^N - f_k(A_N))\psi\|^2 = \sum_{n=k}^{\infty} |c_n - f(\lambda_n)|^2 |\langle \chi_n^N, \psi \rangle|^2 \leq 2M \sum_{n=k}^{\infty} |\langle \chi_n^N, \psi \rangle|^2 \xrightarrow{k \rightarrow \infty} 0 \quad (3.67)$$

since the series $\sum_{n=0}^{\infty} |\langle \chi_n^N, \psi \rangle|^2$ converges and $f_k(A_N)$, therefore, strongly converges to \tilde{J}^N .

Similarly $f_k(A_D)$ strongly converges to J^D . The function f_k is continuous on $(1, \lambda_1)$, so according to Weierstrass theorem it can be uniformly approximated by some polynomial q_k :

$$\max_{x \in [1, \lambda_1]} |f_k(x) - q_k(x)| < \epsilon_k. \quad (3.68)$$

Then it holds for $q_k(A_N)$

$$\|(f_k(A_N) - q_k(A_N))\psi\|^2 = \sum_{n=1}^{\infty} |f(\lambda_n) - p(\lambda_n)|^2 |\langle \chi_n^N, \psi \rangle|^2 \leq \epsilon_k^2 \sum_{n=0}^{\infty} |\langle \chi_n^N, \psi \rangle|^2 = \epsilon_k^2 \|\psi\|^2, \quad (3.69)$$

and analogously

$$\|(f_k(A_D) - q_k(A_D))\psi\|^2 \leq \epsilon_k^2 \|\psi\|^2. \quad (3.70)$$

If we choose ϵ_k such that $\epsilon_k \rightarrow 0$, then for any $\psi \in \mathcal{H}$:

$$\|(\tilde{J}^N - q_k(A_N))\psi\| \leq \|(J^N - f_k(A_N))\psi\| + \epsilon_k \|\psi\| \rightarrow 0. \quad (3.71)$$

so $q_k(A_N)$ strongly converges to \tilde{J}^N and similarly $q_k(A_D)$ strongly converges to \tilde{J}^D . From (3.68) and (3.66) it follows that

$$m - \epsilon < \{\tilde{c}_n\} < M + \epsilon \quad (3.72)$$

so if we choose $\epsilon < m$, $\{\tilde{c}_n\}$ will satisfy (3.2). \square

Using Corollary 3.6, any metric operator θ_α can be written as

$$\theta_\alpha = c_0^\alpha T_1^\alpha + J_N^\alpha (I + T_2^\alpha) + J_D^\alpha T_4. \quad (3.73)$$

According to Proposition 3.7, there exists a sequences of operators of type (3.58) such that

$$J_N^\alpha = s\text{-}\lim_{k \rightarrow \infty} J_{p_k}^N, \quad (3.74)$$

$$J_D^\alpha = s\text{-}\lim_{k \rightarrow \infty} J_{p_k}^D. \quad (3.75)$$

Then, using Theorem 3.6,

$$\theta_k = c_0 T_1 + J_{p_k}^N (I + T_2) + J_{p_k}^D T_4, \quad (3.76)$$

is a series a metric operators, which strongly converges to the metric operator θ_α . Summarizing:

Theorem 3.8. *The set of metric operators of the form*

$$\theta_\alpha = c_0^\alpha T_1^\alpha + J_q^N (I + T_2^\alpha) + J_q^D T_4^\alpha, \quad (3.77)$$

where J_q^N, J_q^D are operators (3.58) with q any polynomial satisfying (3.56) and c_0 any positive number, is dense in strong topology in the set of all metric operators.

4 Examples of metric operators

In this section we use Theorem 3.6 to find explicit formulas for two different metric operators.

4.1 Constant sequence $\{c_n\}$

The simplest sequence satisfying (3.2) for which operator J^N can be summed up is a constant sequence:

$$c_n = c, \quad \forall n \geq 0. \quad (4.1)$$

In this case both J^N and J^D can be summed up trivially:

$$J^N = J^D = c \quad (4.2)$$

and from Corollary 3.6 we immediately get the following expression for metric operator:

$$\eta_\alpha = c (I + K_\alpha^1), \quad (4.3)$$

where K_1 is an integral operator with the following kernel:

$$\begin{aligned} \mathcal{K}_1(x, y) = & \frac{1}{2a} \left(e^{i\alpha(y-x)} - 1 \right) + \frac{i\alpha}{2a}(y-x) - \frac{\alpha^2}{2a}xy + \frac{\alpha^2 a}{2} \\ & + \left(i\alpha - \frac{\alpha^2}{2}(x-y) \right) \text{sgn}(x-y). \end{aligned} \quad (4.4)$$

For $c = 1$ this operator corresponds to the metric operator from papers [21] and [20]. The only difference is that here we consider Hilbert space $L^2((-a, a))$ instead of space $L^2((0, d))$, so operator (4.3) is a unitary transformation of that from papers [21] and [20]. In the following we will always consider $c = 1$.

4.2 \mathcal{C} operator

\mathcal{C} operator is such operator that $\mathcal{C}^2 = 1$ and $\mathcal{P}\mathcal{C}$ is a metric operator, so to find a \mathcal{C} operator we have to find a metric operator ω_α such that $(\mathcal{P}\omega_\alpha)^2 = I$ (because $\mathcal{P}^{-1} = \mathcal{P}$). We can write the operator ω_α using the series (3.1), then $\mathcal{P}\omega_\alpha$ is

$$\mathcal{P}\omega_\alpha = \sum_{j=0}^{\infty} c_j \mathcal{P}\phi_j^\alpha(\phi_j^\alpha, \cdot) = \sum_{j=0}^{\infty} c_j d_j \psi_j^\alpha(\phi_j^\alpha, \cdot), \quad (4.5)$$

where

$$d_j = \begin{cases} \frac{\sin(2\alpha a)}{2\alpha a} & \text{if } j = 0, \\ (-1)^j \frac{k_j^2 - \alpha^2}{k_j^2} & \text{if } j \geq 1. \end{cases} \quad (4.6)$$

Coefficients $\{c_n\}$ can now be determined from the condition $(\mathcal{P}\omega_\alpha)^2 = I$:

$$\begin{aligned} (\mathcal{P}\omega_\alpha)^2 &= \sum_{j=0}^{\infty} c_j d_j \psi_j^\alpha \left(\phi_j^\alpha, \sum_{k=0}^{\infty} c_k d_k \psi_k^\alpha(\phi_k^\alpha, \cdot) \right) \\ &= \sum_{j,k=0}^{\infty} c_j d_j c_k d_k \psi_j^\alpha(\phi_k^\alpha, \cdot)(\phi_j^\alpha, \psi_k^\alpha) = \sum_{j=0}^{\infty} c_j^2 d_j^2 \psi_j^\alpha(\phi_j^\alpha, \cdot) = I. \end{aligned} \quad (4.7)$$

Since $\{\psi_j, \phi_k\}$ is a biorthonormal basis, it follows that $c_j^2 d_j^2 = 1$ and therefore:

$$c_j = \begin{cases} \frac{|2\alpha a|}{|\sin(2\alpha a)|} & \text{if } j = 0, \\ \frac{k_j^2}{|k_j^2 - \alpha^2|} & \text{if } j \geq 1, \end{cases} \quad (4.8)$$

since c_j must be positive. One can easily verify that $\{c_j\}$ indeed satisfies the condition (3.2). We restrict ourselves, for simplicity, to $\alpha \in (-\frac{\pi}{2a}, \frac{\pi}{2a})$. Then $k_j^2 - \alpha^2 > 0$ and also $\frac{2\alpha a}{\sin(2\alpha a)} > 0$. Series J_N^α and J_D^α can be summed up using the functional calculus:

$$J_N^\alpha = \sum_{j=0}^{\infty} \frac{k_j^2}{k_j^2 - \alpha^2} \chi_j^N(\chi_j^N, \cdot) + c_0 \chi_j^N(\chi_j^N, \cdot) \quad (4.9)$$

$$= (-\Delta_N)(-\Delta_N - \alpha^2)^{-1} + c_0 \chi_0^N(\chi_0^N, \cdot) = I + \alpha^2(-\Delta_N - \alpha^2)^{-1} + c_0 \chi_j^N(\chi_j^N, \cdot),$$

$$J_D^\alpha = \sum_{j=1}^{\infty} \frac{k_j^2}{k_j^2 - \alpha^2} \chi_j^D(\chi_j^D, \cdot) = (-\Delta_D)(-\Delta_D - \alpha^2)^{-1} = I + \alpha^2(-\Delta_D - \alpha^2)^{-1}. \quad (4.10)$$

Resolvents of Dirichlet and Neumann Laplacian are integral operators, their kernels are Green's functions of differential equation $-\psi'' - \alpha^2\psi = f$ with Dirichlet resp. Neumann boundary conditions. We again refer to [16, section II-§6] for more details and only present the results:

$$K_N(x, y) = \begin{cases} -\frac{\cos(\alpha(x+a)) \cos(\alpha(y-a))}{\alpha \sin(2\alpha a)} & \text{for } x < y, \\ -\frac{\cos(\alpha(y+a)) \cos(\alpha(x-a))}{\alpha \sin(2\alpha a)} & \text{for } y < x, \end{cases} \quad (4.11)$$

$$K_D(x, y) = \begin{cases} -\frac{\sin(\alpha(x+a)) \sin(\alpha(y-a))}{\alpha \sin(2\alpha a)} & \text{for } x < y, \\ -\frac{\sin(\alpha(y+a)) \sin(\alpha(x-a))}{\alpha \sin(2\alpha a)} & \text{for } y < x. \end{cases} \quad (4.12)$$

After plugging the operators J_N^α and J_D^α into formula (3.50), we find that the metric operator associated with the \mathcal{C} operator has the form

$$\omega_\alpha = I + K_\alpha^{(2)}, \quad \alpha \in (-\frac{\pi}{2a}, \frac{\pi}{2a}), \quad (4.13)$$

where $K_\alpha^{(2)}$ is an integral operator with kernel

$$\mathcal{K}_2(x, y) = \alpha e^{i\alpha(x-y)} (\tan(\alpha a) + i \operatorname{sgn}(x-y)). \quad (4.14)$$

We can now easily find the \mathcal{C} operator by composing the parity operator \mathcal{P} and operator $\theta_\alpha^{(2)}$

$$\mathcal{C} = I + K_\alpha^{(3)}, \quad (4.15)$$

where $K_\alpha^{(3)}$ is an integral operator with the following kernel

$$\mathcal{K}_3(x, y) = \alpha e^{-i\alpha(x+y)} (\tan(\alpha a) - i \operatorname{sgn}(x+y)). \quad (4.16)$$

Note that while there are infinitely many metric operators for this model, the \mathcal{C} operator is unique.

Remark 4.1. If $\alpha \notin (-\frac{\pi}{2a}, \frac{\pi}{2a})$ we can still sum up the series (4.9), (4.10). Let $\alpha^2 \in (k_{j_0}^2, k_{j_0+1}^2)$, then

$$J_N^\alpha = \sum_{j=0}^{\infty} \frac{k_j^2}{k_j^2 - \alpha^2} \chi_j^N(\chi_j^N, \cdot) - 2 \sum_{j=0}^{j_0} \frac{k_j^2}{k_j^2 - \alpha^2} \chi_j^N(\chi_j^N, \cdot) + c_0 \chi_{j_0}^N(\chi_{j_0}^N, \cdot) \quad (4.17)$$

$$= I + \alpha^2(-\Delta_N - \alpha^2)^{-1} + c_0 \chi_{j_0}^N(\chi_{j_0}^N, \cdot) - 2 \sum_{j=0}^{j_0} \frac{k_j^2}{k_j^2 - \alpha^2} \chi_j^N(\chi_j^N, \cdot) \quad (4.18)$$

and similarly for J_D^α .

5 Similar self-adjoint Hamiltonians

To give the physical meaning to our Hamiltonian with some metric θ , we have to choose some decomposition $\theta = \rho^* \rho$ and calculate the operator

$$H_\alpha^F = \rho H_\alpha \rho^{-1}. \quad (5.1)$$

In the following we choose $\rho = \sqrt{\theta}$. Calculating the operator

$$H_\alpha^F = \sqrt{\theta} H_\alpha \sqrt{\theta}^{-1}. \quad (5.2)$$

is in general complicated because even if we have an explicit formula for the metric operator, its square root usually cannot be calculated explicitly. In this section we calculate this self-adjoint Hamiltonian for the metric (4.13). In this case it is possible to find the closed formula for the square root, though the result still contains integrals we cannot calculate explicitly. We also perform a perturbative calculation of the corresponding self-adjoint Hamiltonian for the metric (4.3).

5.1 Metric operator ω_α

To calculate the operator H_α^F one has to find the square root of the metric. One possible way of doing so is using the resolvent formula (see [17, Section VII.3])

$$f(\omega_\alpha) = -\frac{1}{2\pi i} \int_\Gamma f(z)(\omega_\alpha - z)^{-1} dz, \quad (5.3)$$

where Γ is a rectifiable Jordan curve oriented in the positive sense, which encloses the spectrum of ω_α and f is any function such that Γ and the interior of Γ are contained in the domain of analyticity of f . This method can be used for calculating the square root of ω_α , since \sqrt{z} is analytical everywhere except negative real axis and the spectrum of ω_α lies in interval (c, ∞) , where c is some positive number.

To use this formula we have to calculate the resolvent of ω_α .

Proposition 5.1. *The resolvent of ω_α is*

$$(\omega_\alpha - z)^{-1} = -\frac{I}{z-1} - R_\alpha^z, \quad (5.4)$$

where R_α^z is an integral operator with kernel

$$\mathcal{R}_\alpha^z(x, y) = -\frac{2i\alpha}{(z-1)^2} e^{(i\alpha + \frac{2i\alpha}{z-1})(x-y)} (A(z) + \vartheta(x-y)), \quad (5.5)$$

where

$$A(z) = -\left(e^{2I\alpha(1+z)/(1-z)} + 1\right)^{-1}. \quad (5.6)$$

Proof. We first calculate the resolvent of $K_\alpha^{(2)}$, the resolvent of ω_α can then be easily found because

$$(\omega_\alpha - z)^{-1} = \left(K_\alpha^{(2)} - (z-1)\right)^{-1}. \quad (5.7)$$

Finding the resolvent of $K_\alpha^{(2)}$ means solving the equation:

$$\left(K_\alpha^{(2)} - z\right)\psi = \phi, \quad (5.8)$$

for a given function ϕ . For any $\psi \in \mathcal{H}$, $K_\alpha^{(2)}\psi \in W^{1,2}((-a, a))$ and furthermore:

$$\left(K_\alpha^{(2)}\psi\right)' = i\alpha K_\alpha^{(2)}\psi + 2i\alpha\psi. \quad (5.9)$$

Thanks to this relation, it is possible to find the resolvent (and also the spectrum) explicitly. We now restrict ourselves on functions $\psi \in W^{1,2}((-a, a))$; the set of such functions is dense in \mathcal{H} .

The left hand side of equation (5.8) is now in $W^{1,2}((-a, a))$, so the right hand side must also lie in $W^{1,2}((-a, a))$ and we can, therefore, differentiate this equation:

$$i\alpha K_\alpha^{(2)}\psi + 2i\alpha\psi - z\psi' = \phi'. \quad (5.10)$$

and using the equation (5.8)

$$i\alpha\phi + i\alpha z\psi + 2i\alpha\psi - z\psi' = \phi'. \quad (5.11)$$

This is a simple linear differential equation

$$-z\psi' + k(z)\psi = \tilde{\phi}, \quad (5.12)$$

where

$$k(z) = i\alpha z + 2i\alpha, \quad (5.13)$$

$$\tilde{\phi} = \phi' - i\alpha\phi. \quad (5.14)$$

The solution of this equation is

$$\psi(x) = \int_{-a}^x -\frac{2i\alpha}{z^2} e^{\frac{k(z)}{z}(x-y)} \phi(y) dy + e^{\frac{k(z)}{\lambda}x} \left(C + \frac{\phi(-a)}{z} \right) - \frac{\phi(x)}{z}, \quad (5.15)$$

where C is any complex constant. This constant can depend on ϕ and must be determined from equation (5.8). The result is

$$C = -\frac{2i\alpha}{z^2} A(z+1) \int_{-a}^a e^{-\frac{k(z)}{z}y} \phi(y) dy - \frac{\phi(-a)}{z}. \quad (5.16)$$

We have proved that the resolvent of ω_α is equal to (5.4) on the dense subset $W^{1,2}((-a, a))$. Since both resolvent and operator (5.4) are bounded operators, operator (5.4) is indeed equal to the resolvent of ω_α . \square

We can now express $\sqrt{\omega_\alpha}\psi$ as

$$\begin{aligned} \sqrt{\omega_\alpha}\psi &= \frac{1}{2\pi i} \psi \int_{\Gamma} \frac{\sqrt{z}}{z-1} dz \\ &+ \frac{1}{2\pi i} \int_{\Gamma} \sqrt{z} dz \int_{-a}^a R_\alpha^z \psi(y) dy = \frac{1}{2\pi i} \psi \int_{\Gamma} \frac{\sqrt{z}}{z-1} \\ &+ \frac{\alpha}{\pi} \int_{-a}^a \left(\int_{\Gamma} \frac{\sqrt{z}}{(z-1)^2} e^{(i\alpha + \frac{2i\alpha}{z-1})(x-y)} (A(z) + \vartheta(x-y)) dz \right) \psi(y) dy. \end{aligned} \quad (5.17)$$

The interchange of integrals is possible because if we choose some curve Γ :

$$\Gamma(t) : (0, 1) \longrightarrow \mathbb{C}, \quad (5.18)$$

then the function:

$$\frac{\sqrt{\Gamma(t)}}{(\Gamma(t)-1)^2} e^{(i\alpha + \frac{2i\alpha}{\Gamma(t)-1})(x-y)} (A(z) + \vartheta(x-y)) \quad (5.19)$$

is integrable in $L^2((-a, a) \times (0, 1))$. This is true because this function is analytical in z everywhere except points from spectrum, but the curve Γ does not cross spectrum.

The spectrum of ω_α always contains 1 because $K_\alpha^{(2)}$ is a compact operator so it must have 0 in the spectrum and $\sigma(\omega_\alpha) = \sigma(K_\alpha^{(2)}) + 1$. The curve Γ must, therefore, always bound 1. The integral $\int_{\Gamma} \frac{\sqrt{z}}{z-1} dz$ can then be easily calculated using the residue theorem

$$\frac{1}{2\pi i} \int_{\Gamma} \frac{\sqrt{z}}{z-1} dz = 1. \quad (5.20)$$

We were, however unable to calculate the integral:

$$\int_{\Gamma} \frac{\sqrt{z}}{(z-1)^2} e^{(i\alpha + \frac{2i\alpha}{z-1})(x-y)} (A(z) + \vartheta(x-y)) dz \quad (5.21)$$

because it contains infinitely many poles. We can still use the formula (5.17) to find the similar self-adjoint Hamiltonian, but the result also contains integrals, which we do not know how to calculate explicitly.

Theorem 5.2. Operator $H_\alpha^F = \sqrt{\omega_\alpha} H_\alpha \sqrt{\omega_\alpha}^{-1}$ has domain $W^{1,2}((-a, a))$ with boundary conditions

$$\phi'(a) = - \int_{-a}^a \bar{f}^+(y) \phi(y) dy \quad (5.22)$$

$$\phi'(-a) = - \int_{-a}^a \bar{f}^-(y) \phi(y) dy \quad (5.23)$$

and it acts as

$$(H_\alpha^F \phi)(x) = -\phi''(x) + f^+(x)\phi(a) - f^-(x)\phi(-a) + (G\phi)(x), \quad (5.24)$$

where

$$f^+(x) = -\frac{i2\alpha^2}{\pi} \left(\int_{\Gamma} \frac{1}{z-1} f(x, a; z) A(z) dz \right), \quad (5.25)$$

$$f^-(x) = -\frac{i2\alpha^2}{\pi} \left(\int_{\Gamma} \frac{1}{z-1} f(x, -a; z) (A(z) + 1) dz \right), \quad (5.26)$$

and G is a bounded self-adjoint integral operator with kernel

$$\begin{aligned} \mathcal{G}(x, y) &= \frac{\alpha^3}{\pi} \int_{\Gamma} \left(1 + \frac{2}{z-1} \right)^2 g(x, y; z) (A(z) + \vartheta(x-y)) dz \\ &\quad + \left(\frac{\alpha}{\pi} \int_{\Gamma} f(x, a; z) A(z) dz \right) \bar{f}^+(y) \\ &\quad - \left(\frac{\alpha}{\pi} \int_{\Gamma} f(x, -a; z) (A(z) + 1) dz \right) \bar{f}^-(y) \\ &+ \frac{2\alpha^3}{\pi} \int_{\Gamma} \left(\frac{1}{z-1} + \frac{2}{(z-1)^2} \right) f(x, y; z) (A(z) + \vartheta(x-y)) dz \\ &\quad + \frac{\alpha^3}{2\pi} \int_{\Gamma} f(x, y; z) (A(z) + \vartheta(x-y)) dz \\ &\quad + \frac{\alpha^4}{\pi^2} \int_{-a}^a \left(\int_{\Gamma} f(x, y'; z) (A(z) + \vartheta(x-y')) dz \right) \\ &\quad \cdot \left(\int_{\Gamma} \left(1 + \frac{2}{z-1} \right)^2 g(y', y; z) (A(z) + \vartheta(y'-y)) dz \right) dy'. \end{aligned} \quad (5.27)$$

The functions f and g are given by:

$$f(x, y; z) = \frac{\sqrt{z}}{(z-1)^2} e^{(i\alpha + \frac{2i\alpha}{z-1})(x-y)}, \quad (5.28)$$

$$g(x, y; z) = \frac{1}{\sqrt{z}(z-1)^2} e^{(i\alpha + \frac{2i\alpha}{z-1})(x-y)}. \quad (5.29)$$

Proof. We first have to find the domain of H_α^F , which is given by condition:

$$\phi \in \text{Dom}(H_\alpha^F) \Leftrightarrow \sqrt{\omega_\alpha}^{-1} \phi \in \text{Dom}(H_\alpha). \quad (5.30)$$

or equivalently

$$\text{Dom}(H_\alpha^F) = \sqrt{\omega_\alpha} \text{Dom}(H_\alpha). \quad (5.31)$$

The operator $\sqrt{\omega_\alpha}^{-1}$ can be calculated similarly as $\sqrt{\omega_\alpha}$.

$$\sqrt{\omega_\alpha}^{-1} = I + \frac{2i\alpha}{2\pi i} \int_{-a}^a \left(\int_\Gamma g(x, y; z)(A(z) + \vartheta(x - y)) dz \right) \psi(y). \quad (5.32)$$

It follows from (5.31) that $\text{Dom}(H_\alpha^F) \subset W^{2,2}((-a, a))$. The boundary conditions have to be determined from (5.30). If $\phi \in \text{Dom}(H_\alpha^F)$, then it must hold that

$$\left(\sqrt{\omega_\alpha}^{-1} \phi \right)'(-a) + i\alpha \sqrt{\omega_\alpha}^{-1}(-a) = \left(\sqrt{\omega_\alpha}^{-1} \phi \right)'(a) + i\alpha \sqrt{\omega_\alpha}^{-1}(a) = 0. \quad (5.33)$$

The derivative of $(\sqrt{\omega_\alpha}^{-1} \phi)$ is:

$$(\sqrt{\omega_\alpha}^{-1} \phi)' = \phi' + \frac{\alpha}{\pi} \int_\Gamma \frac{d}{dx} \left(\int_{-a}^a g(x, y; z)(A(z) + \vartheta(x - y)) \phi(y) dy \right) dz. \quad (5.34)$$

The interchange of differentiation and integration is justified because both $\int_{-a}^a g(x, y; z)(A(z) + \vartheta(x - y)) \phi(y) dy$ and its derivative are continuous functions of (x, z) . Using Lemma 3.4

$$\begin{aligned} (\sqrt{\omega_\alpha}^{-1} \phi)'(x) &= \phi' - i\alpha \phi \\ &+ \frac{\alpha}{\pi} \int_{-a}^a \left(\int_\Gamma \left(i\alpha + \frac{2i\alpha}{z-1} \right) g(x, y; z)(A(z) + \vartheta(x - y)) dz \right) \phi(y) dy \end{aligned} \quad (5.35)$$

because $g(x, x, z) = \frac{1}{\sqrt{z(z-1)^2}}$ and because from the residue theorem it follows that:

$$\frac{\alpha}{\pi} \int_\Gamma \frac{1}{\sqrt{z(z-1)^2}} = -i\alpha. \quad (5.36)$$

From (5.33) we find that boundary conditions of H_α^F are:

$$\phi'(a) = \int_{-a}^a g^+(y) \phi(y) dy, \quad (5.37)$$

$$\phi'(-a) = \int_{-a}^a g^-(y) \phi(y) dy, \quad (5.38)$$

where

$$g^+(y) = -\frac{2i\alpha^2}{\pi} \int_\Gamma \left(1 + \frac{1}{z-1} \right) g(a, y; z)(A(z) + 1) dz, \quad (5.39)$$

$$g^-(y) = -\frac{2i\alpha^2}{\pi} \int_\Gamma \left(1 + \frac{1}{z-1} \right) g(-a, y; z) A(z) dz. \quad (5.40)$$

We now calculate $H_\alpha \sqrt{\omega_\alpha}^{-1}$ by differentiating (5.35)

$$\begin{aligned} H_\alpha \sqrt{\omega_\alpha}^{-1} \phi &= -\phi'' + i\alpha \phi' + \frac{1}{2} \alpha^2 \phi \\ &- \frac{\alpha}{\pi} \int_{-a}^a \left(\int_\Gamma \left(i\alpha + \frac{2i\alpha}{z-1} \right)^2 g(x, y; z)(A(z) + \vartheta(x - y)) dz \right) \psi(y) dy. \end{aligned} \quad (5.41)$$

To finish the calculation of H_α^F we have to calculate

$$\begin{aligned}
& \frac{i\alpha^2}{\pi} \int_{-a}^a \left(\int_{\Gamma} f(x, y; z)(A(z) + \vartheta(x - y)dz) \right) \phi'(y)dy \\
&= \frac{i\alpha^2}{\pi} \left[\left(\int_{\Gamma} f(x, y; z)(A(z) + \vartheta(x - y)dz) \right) \phi(y) \right]_{-a}^a \\
&+ \frac{i\alpha^2}{\pi} \int_{-a}^a \left(\int_{\Gamma} \left(i\alpha + \frac{2i\alpha}{z-1} \right) f(x, y; z)(A(z) + \vartheta(x - y)dz) \right) \phi(y)dy. \quad (5.42) \\
&\quad + \frac{i\alpha^2}{\pi} \phi(x) \int_{\Gamma} \frac{\sqrt{z}}{(z-1)^2} dz.
\end{aligned}$$

The last term can be calculated using the residue theorem

$$\frac{i\alpha^2}{\pi} \phi(x) \int_{\Gamma} \frac{\sqrt{z}}{(z-1)^2} dz = -\alpha^2 \phi. \quad (5.43)$$

Similarly

$$\begin{aligned}
& -\frac{\alpha}{\pi} \int_{-a}^a \left(\int_{\Gamma} f(x, y; z)(A(z) + \vartheta(x - y)dz) \right) \phi''(y)dy \\
&= -i\alpha\phi' + \frac{\alpha^2}{2}\phi - \frac{\alpha}{\pi} \left[\int_{\Gamma} f(x, y; z)\phi'(y) \right]_{-a}^a \\
&\quad - \frac{\alpha}{\pi} \left[\int_{\Gamma} \left(i\alpha + \frac{2i\alpha}{z-1} \right) f(x, y; z)\phi(y) \right]_{-a}^a \quad (5.44) \\
&-\frac{\alpha}{\pi} \int_{-a}^a \left(\int_{\Gamma} \left(i\alpha + \frac{2i\alpha}{z-1} \right)^2 f(x, y; z)(A(z) + \vartheta(x - y)dz) \right) \phi(y)dy.
\end{aligned}$$

It remains to prove that the boundary conditions have the form (5.22) and (5.23) and that G is a self-adjoint operator. To prove that we will find the sesquilinear form associated with the operator H_α^F , which must be symmetric and show that it is symmetric only if the boundary conditions have the desired form and G is self-adjoint. We define a sesquilinear form by

$$\begin{aligned}
h_\alpha^F(\phi, \psi) &= (\phi', \psi') - \psi(a) \int_{-a}^a \bar{g}^+(y)\bar{\phi}(y)dy + \psi(-a) \int_{-a}^a \bar{g}^-(y)\bar{\phi}(y)dy \\
&+ \bar{\phi}(a) \int_{-a}^a \bar{f}^+(y)\psi(y)dy - \bar{\phi}(-a) \int_{-a}^a \bar{f}^-(y)\psi(y)dy + (\phi, G\psi). \quad (5.45)
\end{aligned}$$

and set $D(h_\alpha^F) = W^{1,2}((-a, a))$. Using integration by parts, it is easy to verify that

$$h_\alpha^F(\phi, \psi) = (H_\alpha^F \phi, \psi), \quad \forall \psi \in D(H_\alpha^F), \forall \phi \in D(h_\alpha^F). \quad (5.46)$$

Let

$$h_0(\phi, \psi) = (\phi', \psi'), \quad D(h_0) = W^{1,2}((-a, a)). \quad (5.47)$$

Using the following lemma it is straightforward to show that the form $h_\alpha^F - h_0$ is h_0 -bounded with h_0 -bound equal to 0. The form h_α^F is then closed and sectorial because the form h_0 is closed and sectorial (see [19, VI.-§1, Theorem 1.33]).

Lemma 5.3. Let $\phi \in W^{1,2}((-a, a))$ and let f be a function from $L^2((-a, a)) \cap L^1((-a, a))$, then

$$|\phi(x) \int_{-a}^a f(y)\phi(y)dy| \leq C\|f\|_1 \left((\epsilon + 1)\|\phi\|^2 + \frac{1}{\epsilon}\|\phi'\|^2 \right) \quad (5.48)$$

for any $x \in [-a, a]$ and some constant C .

Proof. Let $v(y)$ be a linear function, such that $v(-a) = 0$ and $v(x) = 1$, then

$$|\phi(x)|^2 = \int_{-a}^x (|\phi(y)|^2 v(y))' dy. \quad (5.49)$$

Using this expression and inequality

$$2ab \leq \frac{1}{\epsilon}a^2 + \epsilon b^2, \quad \forall \epsilon > 0, \quad (5.50)$$

we find that for any $\epsilon > 0$:

$$\begin{aligned} |\phi(x)|^2 &\leq \int_{-a}^a (|\phi(y)|^2 v(y))' dy = 2\text{Re} \left(\int_{-a}^a \phi'(y) \overline{\phi(y)} v(y) dy \right) + \int_{-a}^a |\phi(y)|^2 v'(y) dy \\ &\leq C(2(\phi, \phi') + \|\phi\|^2) \leq C(2\|\phi\| \|\phi'\| + \|\phi\|^2) \leq C \left((\epsilon + 1)\|\phi\|^2 + \frac{1}{\epsilon}\|\phi'\|^2 \right), \end{aligned}$$

where $C = \max\{v', 1\}$. Using this inequality:

$$|\phi(\pm a) \int_{-a}^a f(y)\phi(y)dy| \leq \|\phi\|_\infty^2 \|f\|_1 \leq C\|f\|_1 \left((\epsilon + 1)\|\phi\|^2 + \frac{1}{\epsilon}\|\phi'\|^2 \right), \quad (5.51)$$

where $\|\phi\|_1$ denotes the $L^1((-a, a))$ norm and $\|\phi\|_\infty$ denotes the supremum norm:

$$\|\phi\|_\infty = \sup_{x \in [-a, a]} \phi(x). \quad (5.52)$$

□

According to first representation theorem there exists a densely defined m-sectorial operator uniquely determined by the condition (5.46). It is self-adjoint if and only if the form is symmetric (see [19, Section VI.-§2.1]). Since we know that the Hamiltonian H_α^F is self-adjoint the form h_α^F must be symmetric. We restrict ourselves on $\phi, \psi \in C_0^\infty((-a, a))$ and from the symmetricity of h_α^F we find that

$$(\phi, G\psi) = (G\phi, \psi), \quad \forall \phi, \psi \in C_0^\infty. \quad (5.53)$$

Since $C_0^\infty((-a, a))$ is a dense set in \mathcal{H} and G a bounded operator, G must be self-adjoint. To finish the proof we can choose for example any $\phi \in W^{1,2}((-a, a))$ such that $\phi(-a) = 0$ and $\phi(a) \neq 0$ and $\psi \in C_0^\infty$ to find that $\bar{f}^+(x) = -g^+(x)$. Similarly by choosing $\phi \in W^{1,2}((-a, a))$ such that $\phi(a) = 0$ and $\phi(-a) \neq 0$ we find that $\bar{f}^-(x) = -g^-(x)$. □

Corollary 5.4. *The sesquilinear form associated with the operator H_α^F is given by*

$$\begin{aligned} h_\alpha^F(\phi, \psi) &= (\phi', \psi') + \psi(a) \int_{-a}^a f^+(y) \bar{\phi}(y) dy - \psi(-a) \int_{-a}^a f^-(y) \bar{\phi}(y) dy \\ &+ \bar{\phi}(a) \int_{-a}^a \bar{f}^+(y) \psi(y) dy - \bar{\phi}(-a) \int_{-a}^a \bar{f}^-(y) \psi(y) dy + (\phi, H\psi) \end{aligned} \quad (5.54)$$

with domain $W^{1,2}((-a, a))$.

This result can be used to easily find approximations of H_α^F for small values of α . To do that one just have to expand functions f and A in the powers of α and consider only first few terms. The integrals (5.25), (5.26) and (5.27) can then be easily calculated using the residue theorem as the integrands then have only one pole. The result is, up to sixth order in α :

$$\tilde{H}_\alpha^F \psi(x) = -\psi''(x) + \tilde{f}(x)(\psi(a) + \psi(-a)), \quad (5.55)$$

$$\psi'(\pm a) = \mp \int_{-a}^a \tilde{f} \psi(y) dy, \quad (5.56)$$

$$\tilde{f}(x) = \frac{1}{768} \alpha^2 (192 + 5a^4 \alpha^4 - 24\alpha^2 x^2 + \alpha^4 x^4 - 6a^2 \alpha^2 (-4 + \alpha^2 x^2)). \quad (5.57)$$

The following proposition shows that \tilde{H}_α^F is a self-adjoint operator and that it indeed is a good approximation of H_α^F . Note that even though we do the proofs for the approximation taken up to sixth order in α , the generalizations to different orders is straightforward.

Proposition 5.5. *Let A be an operator on \mathcal{H} defined by*

$$A\psi(x) = -\psi'' + f(x)(\psi(a) + \psi(-a)) \quad (5.58)$$

$$D(A) = \{\psi \in W^{2,2}((-a, a)) \mid \psi'(\pm a) = \mp \int_{-a}^a \bar{f} \psi(y) dy\}, \quad (5.59)$$

where f is any function from $L^2((-a, a))$. Then A is a densely defined self-adjoint operator.

Proof. To show that the operator A is self-adjoint, we will find its associated sesquilinear form and show that the self-adjoint operator corresponding to this form is the operator A . Very similar approach could be used to show the self-adjointness directly from the definition, but we would then have to prove that the domain of A is a dense set.

Using integration by parts, we find that for any $\psi \in W^{1,2}((-a, a))$, $\phi \in D(A)$:

$$\begin{aligned} (A\phi, \psi) &= (\phi', \psi') + (\psi(-a) + \psi(a)) \int_{-a}^a f(y) \bar{\phi}(y) dy \\ &+ (\bar{\phi}(-a) + \bar{\phi}(a)) \int_{-a}^a \bar{f}(y) \psi(y) dy. \end{aligned} \quad (5.60)$$

This leads us to defining a sesquilinear form h , which acts as right hand side of this equation and has domain $W^{1,2}((-a, a))$.

The form h is obviously symmetric. It is also closed; the proof is precisely the same as the proof of closedness of the form (5.45). Then there exists a unique densely defined self adjoint operator \tilde{A} such that $h(\phi, \psi) = (\tilde{A}\phi, \psi)$ (see [19, VI-§2, Theorem 2.1]). The domain of this operator is given by

$$\phi \in D(\tilde{A}) \Leftrightarrow \exists \varphi \in D(h); \forall \psi \in D(h); h(\phi, \psi) = (\varphi, \psi). \quad (5.61)$$

and it acts as $\tilde{A}\phi = \varphi$. To determine $D(\tilde{A})$ we first restrict ourselves on functions ψ such that

$$\psi(-a) = 0 \wedge \psi(a) = \int_{-a}^a \psi' = 0 \wedge \int_{-a}^a \bar{f}(y)\psi(y)dy = - \int_{-a}^a \left(\int_{-a}^x \bar{f}(y)dy \right) \psi' = 0. \quad (5.62)$$

Let $\phi \in D(\tilde{A})$, then there exists φ such that

$$(\varphi, \psi) = \tilde{h}_\alpha^P(\phi, \psi) = (\phi', \psi'), \quad (5.63)$$

for all ψ satisfying (5.62). Since $\varphi \in L^2((-a, a))$, the integral $\int_{-a}^x \varphi(y)dy$ exists. Therefore:

$$(\phi', \psi') = (\varphi, \psi) = - \left(\int_{-a}^x \varphi(y)dy, \psi' \right) \Rightarrow \quad (5.64)$$

$$\left(\phi' + \int_{-a}^x \varphi(y)dy, \psi' \right) = 0. \quad (5.65)$$

It is easy to show that the set of all ψ' , where ψ satisfies (5.62) is in fact the set of all functions from \mathcal{H} , which are orthogonal to 1 and $\int_{-a}^x f(y)dy$. Then it follows from (5.65) that $\phi' + \int_{-a}^x \varphi(y)dy$ is orthogonal to all function orthogonal to 1 and $\int_{-a}^x f(y)dy$ and it must be, therefore, their linear combination:

$$\phi'(x) = - \int_{-a}^x \varphi(y)dy + A + B \int_{-a}^x f(y)dy. \quad (5.66)$$

This is an absolutely continuous function and its derivative is:

$$\phi'' = -\varphi + Bf. \quad (5.67)$$

Since this is a function from \mathcal{H} , ϕ is in $W^{2,2}((-a, a))$. We now consider any $\psi \in D(\tilde{h}_\alpha^P)$ and use integration by parts:

$$\begin{aligned} (\varphi, \psi) &= \tilde{h}_\alpha^P(\phi, \psi) = -(\phi'', \psi) + \bar{\phi}'(a)\psi(a) - \bar{\phi}'(-a)\psi(-a) \\ &+ (\psi(-a) + \psi(a)) \int_{-a}^a f(y)\bar{\phi}(y)dy + (\bar{\phi}(-a) + \bar{\phi}(a)) \int_{-a}^a \bar{f}(y)\psi(y)dy. \end{aligned} \quad (5.68)$$

Using (5.67) we find the following equality:

$$\begin{aligned} 0 &= -\bar{B} \int_{-a}^a \bar{f}(y)\psi(y)dy + \bar{\phi}'(a)\psi(a) - \bar{\phi}'(-a)\psi(-a) \\ &+ (\psi(-a) + \psi(a)) \int_{-a}^a f(y)\bar{\phi}(y)dy + (\bar{\phi}(-a) + \bar{\phi}(a)) \int_{-a}^a \bar{f}(y)\psi(y)dy, \end{aligned} \quad (5.69)$$

which must hold for all $\psi \in D(\tilde{h}_\alpha^P)$. If we now choose ψ such that $\psi(-a) = 0$ and $\psi(a) = 0$, we find that

$$\bar{B} = (\bar{\phi}(-a) + \bar{\phi}(a)). \quad (5.70)$$

Similarly by choosing ψ such that $\int_{-a}^a \bar{f}(y)\psi(y)dy = 0$, $\psi(\pm a) = 0$ and $\psi(\mp a) \neq 0$ we see that it must hold

$$\phi'(\pm a) = \mp \int_{-a}^a \bar{f}(y)\phi(y)dy. \quad (5.71)$$

We have thus shown that $D(\tilde{A}) \subset D(A)$ and $\tilde{A}\phi = A\phi$ for all $\phi \in D(\tilde{A})$. It is easy to show that $D(A) \subset D(\tilde{A})$ because for $\phi \in D(A)$

$$\tilde{h}_\alpha^P(\phi, \psi) = (A\phi, \psi), \quad \forall \psi \in W^{1,2}((-a, a)). \quad (5.72)$$

and, therefore, $A = \tilde{A}$. □

We will prove that the operator \tilde{H}_α^F is indeed a good approximation of H_α^F . Since these are unbounded operator we have to prove that their resolvents are close.

Proposition 5.6. *Resolvents of H_α^F and \tilde{H}_α^F satisfy*

$$\|(H_\alpha^F + k)^{-1} - (\tilde{H}_\alpha^F + k)^{-1}\| < C\alpha^7, \quad (5.73)$$

where C is a constant and k is a real number not in the spectrum of H_α^F and \tilde{H}_α^F for α in some interval $(-\alpha_0, \alpha_0)$.

Proof. Up to now we have considered $\alpha \in \mathbb{R}$, but the form h_α^F is well defined, closed and sectorial even for complex α . This is true because it is still a bounded perturbation of the form h_0 . We can define H_α^F for complex α as the self-adjoint operator corresponding to h_α^F . $h_\alpha^F(\phi, \psi)$ is holomorphic in α for any $\psi, \phi \in D(h_\alpha^F)$, therefore, H_α^F is a holomorphic family of operators (see [19, VII.-§4]).

Then according to the theorem [19, VII.-§1, Theorem 1.3]), there exists a neighbourhood of 0 such that if k is in the resolvent set of H_0^F then it is also in the resolvent set of H_α^F for α from this neighbourhood and $(H_\alpha^F - k)^{-1}$ is a holomorphic family of operators. Therefore, there exists an interval $\mathcal{I} = [-\alpha_0, \alpha_0]$ such that k is in the resolvent set of H_α^F for $\alpha \in \mathcal{I}$ and $\|(H_\alpha^F - k)^{-1}\|$ is continuous on \mathcal{I} . From now on we will again consider α to be real.

The same also holds for \tilde{H}_α^F because it follows from the proof of Proposition 5.5 that the sesquilinear form associated with the operator \tilde{H}_α^F is given by

$$\begin{aligned} \tilde{h}_\alpha^F(\phi, \psi) &= (\phi', \psi') + (\psi(-a) + \psi(a)) \int_{-a}^a \tilde{f}(y)\bar{\phi}(y)dy \\ &\quad + (\bar{\phi}(-a) + \bar{\phi}(a)) \int_{-a}^a \tilde{f}(y)\psi(y)dy, \end{aligned} \quad (5.74)$$

$$D(\tilde{h}_\alpha^F) = W^{1,2}((-a, a)). \quad (5.75)$$

and it is also analytical in α .

Let $F, G \in \mathcal{H}$, then there exists functions $\psi \in D(H_\alpha)$, $\phi \in D(\tilde{H}_\alpha)$ such that

$$(H_\alpha^F + k)\psi = F, \quad (5.76)$$

$$(\tilde{H}_\alpha^F + k)\phi = G. \quad (5.77)$$

Since both $(H_\alpha^F + k)^{-1}$ and $(\tilde{H}_\alpha^F + k)^{-1}$ are self-adjoint operators we can express the norm (5.73) as

$$\begin{aligned} \|(H_\alpha^F + k)^{-1} - (\tilde{H}_\alpha^F + k)^{-1}\| &= \sup_{F, G \in \mathcal{H}} \frac{|(F, (H_\alpha^F + k)^{-1} - (\tilde{H}_\alpha^F + k)^{-1}G)|}{\|F\| \|G\|} \\ &= \sup_{F, G \in \mathcal{H}} \frac{|((H_\alpha^F + k)^{-1}F, G) - (F, (\tilde{H}_\alpha^F + k)^{-1}G)|}{\|F\| \|G\|} \\ &= \sup_{F, G \in \mathcal{H}} \frac{|((\psi, (\tilde{H}_\alpha^F + k)\phi) - ((H_\alpha^F + k)\psi, \phi))|}{\|F\| \|G\|} \end{aligned} \quad (5.78)$$

Using the forms h_α^F , \tilde{h}_α^F , we can write (5.78) as

$$\|(H_\alpha^F + k)^{-1} - (\tilde{H}_\alpha^F + k)^{-1}\| = \sup_{F, G \in \mathcal{H}} \frac{|(\tilde{h}_\alpha^F(\phi, \psi) - h_\alpha^F(\phi, \psi))|}{\|F\| \|G\|}. \quad (5.79)$$

The numerator has the form

$$\begin{aligned} \tilde{h}_\alpha^F(\phi, \psi) - h_\alpha^F(\phi, \psi) &= \alpha^7 \left(\bar{\phi}(a) \int_{-a}^a \bar{f}_1(y) \psi(y) dy + \bar{\phi}(-a) \int_{-a}^a \bar{f}_2(y) \psi(y) dy \right. \\ &\quad \left. + \psi(a) \int_{-a}^a \bar{f}_3(y) \bar{\phi}(y) dy + \psi(a) \int_{-a}^a \bar{f}_4(y) \bar{\phi}(y) dy + (\phi, G\psi) \right), \end{aligned} \quad (5.80)$$

where f_i and G are functions continuous in α . We will show that

$$|\tilde{h}_\alpha^F(\phi, \psi) - h_\alpha^F(\phi, \psi)| \leq |\alpha|^7 C \|F\| \|G\|. \quad (5.81)$$

We can bound the first two terms in (5.80) by

$$|\bar{\phi}(a) \int_{-a}^a \bar{f}_1(y) \psi(y) dy + \bar{\phi}(-a) \int_{-a}^a \bar{f}_2(y) \psi(y) dy| \leq C_1 \|\phi\|_\infty \|\psi\|, \quad (5.82)$$

where

$$C_1 = \max \left\{ \sup_{\alpha \in \mathcal{I}} \|f_1\|, \sup_{\alpha \in \mathcal{I}} \|f_2\| \right\}. \quad (5.83)$$

C_1 is finite because f_1 and f_2 are continuous in α . We can bound $\|\psi\|$ by

$$\|\psi\| = \|(H_\alpha^F + k)^{-1}F\| \leq \|(H_\alpha^F + k)^{-1}\| \|F\| \leq C_2 \|F\|, \quad (5.84)$$

where

$$C_2 = \sup_{\alpha \in \mathcal{I}} \|(H_\alpha^F + k)^{-1}\|. \quad (5.85)$$

The supremum exists and is finite because $(H_\alpha^F + k)^{-1}$ is a continuous function in α . According to the Sobolev imbedding theorem (see [3, Theorem 5.4]), $\|\phi\|_\infty$ can be bound by $W^{1,2}((-a, a))$ norm:

$$\|\phi\|_\infty \leq C_3 \sqrt{\|\phi\|^2 + \|\phi'\|^2} \leq C_3(\|\phi\| + \|\phi'\|), \quad (5.86)$$

for some constant C_3 . $\|\phi\|$ can be bound in the same way as $\|\psi\|$:

$$\|\phi\| \leq C_4 \|F\|, \quad (5.87)$$

where

$$C_4 = \sup_{\alpha \in \mathcal{I}} \|(\tilde{H}_\alpha^F + k)^{-1}\|. \quad (5.88)$$

To bound also the norm of ϕ' we consider the following

$$|\tilde{h}_\alpha^F(\phi, \phi) + k\|\phi\|^2| = |(\phi, F)| \leq \|\phi\| \|F\| \leq C_4 \|F\|^2 \quad (5.89)$$

and using Lemma 5.3

$$\begin{aligned} |\tilde{h}_\alpha^F(\phi, \phi) + k\|\phi\|^2| &\geq \|\phi'\|^2 - C_5 \left(\frac{1}{\epsilon} \|\phi'\|^2 + (1 + \epsilon) \|\phi\|^2 \right) + k\|\phi\|^2 \\ &= \|\phi'\|^2 \left(1 - \frac{C_5}{\epsilon} \right) + \|\phi\|^2 (k - 1 - \epsilon), \end{aligned} \quad (5.90)$$

for some constant C_5 and any positive ϵ . We now choose $\epsilon > C_5$ and $k > 1 + \epsilon$, then

$$\|\phi'\| \leq C_6 \|F\|, \quad (5.91)$$

where

$$C_6 = \sqrt{\frac{C_4}{1 - \frac{C_5}{\epsilon}}} \quad (5.92)$$

and there, therefore, exists a constant C such that

$$|\bar{\phi}(a) \int_{-a}^a \bar{f}_1(y) \psi(y) dy + \bar{\phi}(-a) \int_{-a}^a \bar{f}_2(y) \psi(y) dy| \leq C \|F\| \|G\|. \quad (5.93)$$

We can show analogously that the same also holds for the term

$$|\psi(a) \int_{-a}^a \bar{f}_3(y) \bar{\phi}(y) dy + \psi(-a) \int_{-a}^a \bar{f}_4(y) \bar{\phi}(y) dy| \quad (5.94)$$

and since G is a bounded operator also for the term $(\phi, G\psi)$.

□

5.2 Metric operator η_α

The resolvent formula (5.3) cannot be used to calculate the square root of the metric operator η_α because we cannot calculate its resolvent explicitly. We instead calculate an approximation of the square root and its inversion perturbatively.

We first expand η_α up to second order in α :

$$\eta_\alpha = I + \alpha L_1 + \alpha^2 L_2 + O(\alpha^3), \quad (5.95)$$

where L_1 and L_2 are integral operators with kernels (respectively):

$$\mathcal{L}_1 = i \operatorname{sgn}(x - y), \quad (5.96)$$

$$\mathcal{L}_2 = x\vartheta(y - x) + y\vartheta(x - y) - \frac{1}{4a}(x^2 + y^2) + \frac{a}{2} - \frac{(x + y)}{2}. \quad (5.97)$$

Using Taylor expansions:

$$\sqrt{1 + x} = 1 + \frac{x}{2} - \frac{x^2}{8} + O(x^3), \quad (5.98)$$

$$\frac{1}{1 - x} = 1 + x + x^2 + O(x^3), \quad (5.99)$$

we find that the square root and its inversion are up to second order equal to:

$$\sqrt{\eta_\alpha} = \rho + O(\alpha^3) = I + \frac{\alpha}{2}L_1 + \frac{\alpha^2}{2}L_2 - \frac{\alpha^2}{8}L_1L_1 + O(\alpha^3) = I + M_1 + O(\alpha^3), \quad (5.100)$$

$$\sqrt{\eta_\alpha}^{-1} = \tilde{\rho} + O(\alpha^3) = I - \frac{\alpha}{2}L_1 - \frac{\alpha^2}{2}L_2 + \frac{3\alpha^2}{8}L_1L_1 + O(\alpha^3) = I + M_2 + O(\alpha^3), \quad (5.101)$$

where M_1, M_2 are integral operators with kernels

$$\begin{aligned} \mathcal{M}_1 = & \left(\frac{i\alpha}{2} + \frac{\alpha^2}{4}(x - y) \right) \operatorname{sgn}(x - y) + \frac{\alpha^2}{2}(y\vartheta(x - y) + x\vartheta(y - x)) \\ & - \frac{\alpha^2}{8a}(x^2 + y^2) - \frac{\alpha^2}{4}(x + y), \end{aligned} \quad (5.102)$$

$$\begin{aligned} \mathcal{M}_2 = & \left(\frac{i\alpha}{2} + \frac{3\alpha^2}{4}(x - y) \right) \operatorname{sgn}(y - x) - \frac{\alpha^2}{2}(y\vartheta(x - y) + x\vartheta(y - x)) \\ & + \frac{\alpha^2}{8a}(x^2 + y^2) + \frac{1}{4}\alpha^2(x + y) + \frac{\alpha^2 a}{2}. \end{aligned} \quad (5.103)$$

Following proposition shows that ρ and $\tilde{\rho}$ are indeed good approximations of $\sqrt{\eta_\alpha}$ resp. $\sqrt{\eta_\alpha}^{-1}$.

Proposition 5.7. *There exist constants C_1, C_2 such that*

$$\|\rho - \sqrt{\eta_\alpha}\| < C_1\alpha^3, \quad (5.104)$$

$$\|\tilde{\rho} - \sqrt{\eta_\alpha}^{-1}\| < C_2\alpha^3. \quad (5.105)$$

for α from some interval $[-\alpha_0, \alpha_0]$.

Proof. If we consider α to be complex, then η_α is a holomorphic family of operators and according to [19, Section VII-§6, Remark 5.6] so is $\sqrt{\eta_\alpha}$. We can, therefore, write

$$\eta_\alpha = \sum_{n=0}^{\infty} \alpha^n K_n, \quad (5.106)$$

$$\sqrt{\eta_\alpha} = \sum_{n=0}^{\infty} \alpha^n \tilde{K}_n, \quad (5.107)$$

where K_n, \tilde{K}_n are bounded operators, which do not depend on α . We can easily show that $\rho^2 - \eta_\alpha$ is of third order in α , then it must hold:

$$I + M_1 = K_0 + \alpha K_1 + \alpha^2 K_2 \quad (5.108)$$

and therefore we can choose some interval $[-\alpha_0, \alpha_0]$ and find a constant C_1 such that

$$\|\rho - \sqrt{\eta_\alpha}\| < C_1 \alpha^3, \quad \forall \alpha \in [-\alpha_0, \alpha_0]. \quad (5.109)$$

Similarly, we can show that $\tilde{\rho}\rho - I$ is of third order in α , then

$$\|\tilde{\rho} - \sqrt{\eta_\alpha}^{-1}\| = \|(\tilde{\rho}\sqrt{\eta_\alpha} - I)\sqrt{\eta_\alpha}^{-1}\| \quad (5.110)$$

$$\leq \|\sqrt{\eta_\alpha}^{-1}\| \|\tilde{\rho}\rho - I\| + \|\sqrt{\eta_\alpha}^{-1}\| \|\tilde{\rho}\| \|\rho - \sqrt{\eta_\alpha}\| \quad (5.111)$$

Both $\|\sqrt{\eta_\alpha}^{-1}\|$ and $\|\tilde{\rho}\|$ can be bound by constant on $[-\alpha_0, \alpha_0]$. \square

We can now approximate the self-adjoint Hamiltonian

$$H_\alpha^P = \sqrt{\eta_\alpha} H_\alpha \sqrt{\eta_\alpha}^{-1} \quad (5.112)$$

by calculating the operator

$$\tilde{H}_\alpha^P = \rho H_\alpha \tilde{\rho}. \quad (5.113)$$

up to second order in α . The calculation is similar to the proof of Theorem 5.2. Let $\phi \in \mathcal{H}$

$$(\tilde{\rho}\phi)' = \phi' - i\alpha\phi + \frac{\alpha^2}{4} \int_x^a \phi(y) dy - \frac{3}{4}\alpha^2 \int_{-a}^x \phi(y) dy + \int_{-a}^a \left(\frac{\alpha^2}{4a} x + \frac{\alpha^2}{4} \right) \phi(y) dy. \quad (5.114)$$

From this it is easy to show that the domain of \tilde{H}_α^P are functions from $W^{2,2}((-a,a))$ satisfying:

$$\phi'(a) = -\frac{\alpha^2}{4} \int_{-a}^a \phi(y) dy, \quad (5.115)$$

$$\phi'(-a) = \frac{\alpha^2}{4} \int_{-a}^a \phi(y) dy. \quad (5.116)$$

Differentiating (5.114):

$$(\tilde{\rho}\phi)'' = \phi'' - i\alpha\phi' - \alpha^2\phi + \frac{\alpha^2}{4} \int_{-a}^a \phi(y) dy. \quad (5.117)$$

Using integration by parts and boundary conditions we can show that:

$$M_1\phi''(x) = i\alpha\phi'(x) + \frac{\alpha^2}{4}\phi(-a) + \frac{\alpha^2}{4}\phi(a) - \frac{\alpha^2}{4a}\int_{-a}^a\phi(y)dy, \quad (5.118)$$

$$-i\alpha M_1\phi'(x) = \alpha^2\phi(x) - \frac{\alpha^2}{2}(\phi(-a) + \phi(a)). \quad (5.119)$$

And thus the operator \tilde{H}_α^P is:

$$\tilde{H}_\alpha^P\phi = -\phi'' + \frac{\alpha^2}{4}(\phi(-a) + \phi(a)) + O(\alpha^3). \quad (5.120)$$

This is a same operator as operator H_α^F taken up to second order in α . According to Proposition 5.5 this is a densely defined self-adjoint operator.

5.2.1 Spectrum of the similar self-adjoint Hamiltonian

In this section we calculate the spectrum of the approximate self-adjoint Hamiltonian \tilde{H}_α^P to see how it differs from the spectrum of the exact self-adjoint Hamiltonian H_α^P . We have to find λ for which the equation

$$-\phi'' + \frac{\alpha^2}{4}(\phi(-a) + \phi(a)) = \lambda\phi, \quad \phi \in D(\tilde{H}_\alpha^P) \quad (5.121)$$

has solution. If ϕ is a solution of this equation then

$$\phi_\pm = \phi(x) \pm \phi(-x) \quad (5.122)$$

is also a solution because

$$-\phi_+'' + \frac{\alpha^2}{4}(\phi_+(-a) + \phi_+(a)) = -\phi(x)'' - \phi(-x)'' + \frac{\alpha^2}{2}(\phi(-a) + \phi(a)) \quad (5.123)$$

$$= \lambda(\phi(x) + \phi(-x)) = \lambda\phi_+(x), \quad (5.124)$$

and similarly

$$-\phi_-'' + \frac{\alpha^2}{4}(\phi_-(-a) + \phi_-(a)) = -\phi''(x) + \phi''(-x) = \lambda(\phi(x) - \phi(-x)) = \lambda\phi_-(x). \quad (5.125)$$

Furthermore if ϕ satisfies boundary conditions (5.115) and (5.116), then also ϕ_\pm satisfies these boundary conditions because

$$\phi_+'(a) = \phi'(a) - \phi'(-a) = \frac{\alpha^2}{2}\int_{-a}^a\phi(y)dy, \quad (5.126)$$

$$\phi_+'(-a) = \phi'(-a) + \phi'(a) = -\frac{\alpha^2}{2}\int_{-a}^a\phi(y)dy, \quad (5.127)$$

and

$$\int_{-a}^a\phi_+(y)dy = \int_{-a}^a\phi(y)dy + \int_{-a}^a\phi(-y)dy = 2\int_{-a}^a\phi(y)dy, \quad (5.128)$$

similarly

$$\phi'_-(a) = \phi'(a) + \phi'(-a) = 0, \quad (5.129)$$

$$\phi'_-(-a) = \phi'(-a) + \phi'(a) = 0, \quad (5.130)$$

and

$$\int_{-a}^a \phi_-(y) dy = 0. \quad (5.131)$$

Because ϕ_+ is an even function and ϕ_- is an odd function, it follows that any eigenfunction of the operator \tilde{H}_α^P can be chosen to be either even or odd. We shall treat these two cases separately.

a) Odd eigenfunctions

If ψ is an odd eigenfunction of \tilde{H}_α^P , then $\psi(a) = -\psi(-a)$ and ψ must satisfy boundary conditions (5.129) and (5.130). ψ is, therefore, an eigenfunction of the Neumann Laplacian. The spectrum of the Neumann Laplacian is

$$\sigma(-\Delta_N) = \{k_n^2\}_{n=0}^\infty \quad (5.132)$$

and the eigenfunctions are given by

$$\chi_j^N = \begin{cases} \frac{1}{\sqrt{2a}} & \text{for } j = 0, \\ \frac{1}{\sqrt{a}} \cos(k_j(x+a)) & \text{for } j \geq 1. \end{cases} \quad (5.133)$$

χ_j^N is odd if j is odd so we find that k_j^2 lies in the spectrum of \tilde{H}_α^P if j is odd. These eigenvalues are also in the spectrum of H_α^P .

a) Even eigenfunctions

Let ψ be an even eigenfunction of \tilde{H}_α^P . We denote

$$c = \frac{\alpha^2}{4}(\psi(-a) + \psi(a)). \quad (5.134)$$

Then ψ must satisfy equation

$$-\psi'' + c = \lambda\psi \quad (5.135)$$

and boundary conditions (5.115), (5.116). Since ψ is even, it suffices if it satisfies one boundary condition, the other one will be satisfied automatically. The general solution of this equation can be written as

$$\psi(x) = C_1 e^{\sqrt{-\lambda}x} + C_2 e^{-\sqrt{-\lambda}x} + \frac{c}{\lambda}. \quad (5.136)$$

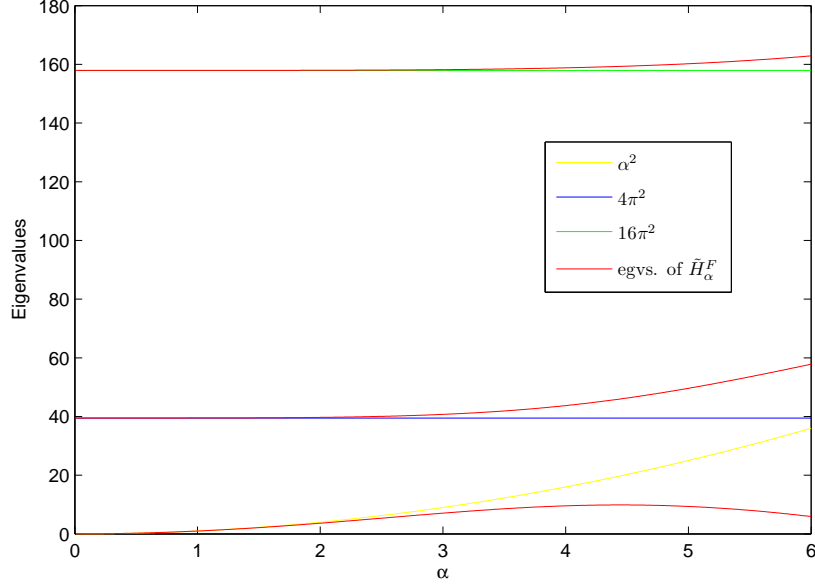


Figure 4: Lowest three solutions of equation (5.138) compared with the corresponding eigenvalues of the exact Hamiltonian H_α^P

Since ψ is even, it must hold that $C_1 = C_2$. From (5.134) we find that

$$c = \frac{\alpha^2}{1 - \frac{\alpha^2}{2\lambda}} \frac{C_1}{2} (e^{\sqrt{-\lambda}a} + e^{-\sqrt{-\lambda}a}). \quad (5.137)$$

From the boundary conditions we get the following equation

$$\left(\sqrt{-\lambda} + \frac{\alpha^2}{2\sqrt{-\lambda}} \right) (e^{\sqrt{-\lambda}a} - e^{-\sqrt{-\lambda}a}) + \frac{\frac{1}{4}\alpha^2 a}{\lambda - \alpha^2/2} (e^{\sqrt{-\lambda}a} + e^{-\sqrt{-\lambda}a}) = 0. \quad (5.138)$$

If λ solves this equation then it is an eigenvalue of \tilde{H}_α^P . We found the lowest three solutions of this equation numerically. Figure 4 shows how they depend on α . For small α they are very similar to the eigenvalues α^2, k_2^2, k_4^2 of the exact Hamiltonian H_α^P .

Conclusions

Non-self-adjoint operators can be used to describe observables in quantum mechanics, if there exists a metric operator. We studied a simple \mathcal{PT} -symmetric non-self-adjoint one-parametric class of Hamiltonians H_α with real spectrum. The metric operator associated with this Hamiltonians was already found in paper [21]. We examined the form of a general metric operator associated with this Hamiltonian and we showed that such metric operators are connected to the metric operators of a simple self-adjoint operator—the Neumann Laplacian. We presented a method for explicitly finding dense subset (in strong topology) of all metric operators.

We used this results to find two different metric operators and the \mathcal{C} -operator. For one of these metric operators we used the resolvent formula to find its square root and then calculated the corresponding similar self-adjoint Hamiltonian. This result is not explicit because we were unable to find calculate certain integrals, but it can be used to find explicit approximation for small values of α , which corresponds to the case when H_α is a small perturbation of self-adjoint operator. We showed that this approximation is self-adjoint and that it is close to the exact self-adjoint Hamiltonian in a norm-resolvent sense. This Hamiltonian is a self-adjoint operator on L^2 space and it can, therefore, have a direct physical meaning. We also did a perturbative calculation of the square root and of the corresponding self-adjoint Hamiltonian for the other metric operator. We found that these two self-adjoint Hamiltonians are the same up to second order in α .

A Some topics from functional analysis

Self-adjoint operators

Let A be a bounded operator on some Hilbert space \mathcal{H} , its adjoint A^* is defined by

$$(\phi, A\psi) = (A^*\phi, \psi), \quad \forall \phi, \psi \in \mathcal{H}. \quad (\text{A.1})$$

This is good definition because there exists a unique operator, which satisfy this relation. If A is unbounded then a more complicated definition is needed. Let A be a densely defined operator, its adjoint A^* is given by

$$\phi \in D(A^*) \Leftrightarrow \exists \varphi; \forall \psi \in D(A); (\phi, A\psi) = (\varphi, \psi), \quad (\text{A.2})$$

$$A^*\phi = \varphi. \quad (\text{A.3})$$

A is called self-adjoint if $A = A^*$ and symmetric if $A \subset A^*$. In physics the term Hermitian is usually used for self-adjoint operators and often the difference between bounded and unbounded operators is neglected.

Stone's theorem

For proofs and more informations see e.g. [34, Section VIII.4]. Let A be a self-adjoint operator on some Hilbert space \mathcal{H} . We can define exponential of such operator using the spectral theorem:

$$A = \int \lambda dE_A(\lambda), \quad (\text{A.4})$$

$$e^{iAt} = \int e^{i\lambda t} dE_A(\lambda), \quad t \in \mathbb{R}. \quad (\text{A.5})$$

e^{iAt} is for any t unitary and it satisfies:

$$U(t+s) = U(t)U(s). \quad (\text{A.6})$$

The map $s \rightarrow U(s)$ is strongly continuous and furthermore:

$$\lim_{h \rightarrow 0} \frac{U(t+h)\psi - U(t)\psi}{h} = iAU(t)\psi, \quad \forall \psi \in D(A). \quad (\text{A.7})$$

Definition A.1. The set $\{U(s), s \in \mathbb{R}\}$ of unitary operators is called a **strongly continuous one-parameter unitary group** if the map $s \rightarrow U(s)$ is strongly continuous and if it satisfies (A.6).

Theorem A.2 (Stone's theorem). *Let $U(t)$ be a strongly continuous one-parameter unitary group, then there exists a self-adjoint operator A such that*

$$U(t) = e^{iAt}. \quad (\text{A.8})$$

Irreducible operator sets

For proofs and more informations see [13, Section 6.7].

Definition A.3. Let \mathcal{A} be a set of operators on some Hilbert space \mathcal{H} . It is called **reducible** if there exists a nontrivial projection E (here projection is a self-adjoint operator such that $E^2 = E$) such that for every $A \in \mathcal{A}$:

$$ED(A) \subset D(A), \quad (\text{A.9})$$

$$AE\mathcal{H} \subset E\mathcal{H}, \quad A(I - E)\mathcal{H} \subset (I - E)\mathcal{H}. \quad (\text{A.10})$$

If no such projection exists, \mathcal{A} is called **irreducible**.

Definition A.4. Let \mathcal{A} be a set of operators on some Hilbert space \mathcal{H} . Its **commutant** is the set of all bounded operators B such that :

$$BA \subset AB, \quad A \in \mathcal{A}. \quad (\text{A.11})$$

Theorem A.5. Let \mathcal{A} be a set of operators such that for any $A \in \mathcal{A}$ one of the following holds:

1. A is self-adjoint
2. A is bounded and $A^* \in \mathcal{A}$

Then \mathcal{A} is irreducible if and only if its commutant is the set $\{cI | c \in \mathbb{C}\}$.

Corollary A.6. Any self-adjoint operator is reducible.

Proof. Any bounded function of self-adjoint operator lies in its commutant. \square

Dirichlet and Neumann Laplacians

Dirichlet and Neumann Laplacians, denoted by $-\Delta_D$ and $-\Delta_N$ respectively are operators on $L^2((-a, a))$, which both act as minus second derivative, but have different boundary conditions

$$D(-\Delta_D) = \{\varphi \in W^{1,2}((-a, a)) | \varphi(-a) = \varphi(a) = 0\}, \quad (\text{A.12})$$

$$D(-\Delta_N) = \{\varphi \in W^{1,2}((-a, a)) | \varphi'(-a) = \varphi'(a) = 0\}. \quad (\text{A.13})$$

They are self-adjoint operators and they both have purely point spectrum, thus they can be decomposed as

$$-\Delta_D = \sum_{j=0}^{\infty} \lambda_j^D \chi_j^D(\chi_j^D, \cdot) \quad -\Delta_N = \sum_{j=0}^{\infty} \lambda_j^N \chi_j^N(\chi_j^N, \cdot), \quad (\text{A.14})$$

where λ_j^D and χ_j^D resp. λ_j^N and χ_j^N denotes eigenvalues and eigenfunctions of Dirichlet resp. Neumann Laplacian. They are given by

$$\begin{aligned}\lambda_j^D &\equiv k_j^2 = \left(\frac{j\pi}{2a}\right)^2, & j \geq 1 \\ \chi_j^D &= \sqrt{\frac{1}{a}} \sin(k_j(x+a)), & j \geq 1.\end{aligned}\tag{A.15}$$

for the Dirichlet Laplacian, resp.

$$\lambda_j^N \equiv k_j^2 = \left(\frac{j\pi}{2a}\right)^2, \quad j \geq 0\tag{A.16}$$

$$\chi_j^N = \begin{cases} \sqrt{\frac{1}{2a}} & \text{for } j = 0, \\ \sqrt{\frac{1}{a}} \cos(k_j(x+a)) & \text{for } j \geq 1.\end{cases}\tag{A.17}$$

for the Neumann Laplacian.

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