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Schrödingerovy operátory s nehermitovskými maticovými potenciály

Schrödinger operators with non-Hermitian matrix-valued potentials

Master's Thesis

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- Zadání práce -

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Author's declaration:

I declare that this Master's Thesis is entirely my own work and I have listed all the used sources in the bibliography.

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Název práce:

Schrödingerovy operátory s nehermitovskými maticovými potenciály

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Abstrakt: K formulaci nehermitovské kvantové fyziky je třeba studovat matematický aparát pro nesamosdružené operátory. Konkrétně se zaměříme na Schrödingerův operátor s nehermitovskými maticovými potenciály. Uvažovat maticové potenciály je obzvláště důležité při zahrnutí elektromagnetického pole, jak můžeme vidět na Pauliho operátoru. Hlavním úkolem je korektně definovat Schrödingerův operátor jako součet volného Hamiltoniánu a potenciálu. Bude zajištěna stabilita esenciálního spektra. Nakonec se budeme věnovat spektru bodovému. Odvodíme odhad na vlastní čísla v první dimenzi a vyslovíme podmínku na potenciál, která vylučuje existenci bodového spektra ve třetí dimenzi.

Klíčová slova: Schrödingerův operátor, Pauliho operátor, nehermitovský maticový potenciál, relativně omezené potenciály, stabilita esenciálního spektra, odhad na vlastní čísla

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Abstract: To formulate non-Hermitian quantum physics, it is necessary to study the mathematical apparatus for non-self-adjoint operators. Matrix-valued potentials play a role especially in involving the interaction of a particle spin with an electromagnetic field, as can be seen in the Pauli operator. Specifically, we focus on the Schrödinger operator with non-Hermitian matrix-valued potentials. The main task is to correctly define this operator as the sum of the free Hamiltonian and the potential. We derive conditions for the potential to ensure the stability of the essential spectrum. Finally, we derive an estimate of the eigenvalues in the first dimension and state a condition for the potential that excludes the existence of a point spectrum in the third dimension.

Key words: Schrödinger operator, Pauli operator, non-Hermitian matrix-valued potential, relatively form-bounded potentials, stability of essential spectrum, estimation of eigenvalues

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Notation

- Let \mathcal{H} be a separable complex Hilbert space.
- Inner product is denoted as (\cdot, \cdot) and corresponding norm $\|\cdot\|$.
- $\mathcal{B}(\mathcal{H})$ is the set of bounded linear operators on \mathcal{H} .
- $\mathcal{B}^\infty(\mathcal{H})$ is the set of compact linear operators on \mathcal{H} .
- Let Ω be an open set in \mathbb{R}^d .
- $D(A)$ denotes domain of the linear operator A , $\text{Ran}(A)$ its range and $\text{Ker} A$ its null-space.
- $C(\Omega) := \{\psi : \Omega \rightarrow \mathbb{C} \mid \psi \text{ continuous}\}$.
- $C^k(\Omega) := \{\psi : \Omega \rightarrow \mathbb{C} \mid D^\alpha \psi \in C(\Omega) \text{ for } 0 \leq |\alpha| \leq k\}$.
- $C_0^k(\Omega) := \{\psi \in C^k(\Omega) \mid \text{supp } \psi \text{ is compact}\}$.
- $W^{k,p}(\Omega) := \{\psi \in L^p(\Omega) \mid D^\alpha \psi \in L^p(\Omega) \text{ for } 0 \leq |\alpha| \leq k\}$.
- $\|\psi\|_{W^{k,p}(\Omega)} := \left(\sum_{i=0}^k \|\psi^{(i)}\|_p^p \right)^{\frac{1}{p}}$.
- $W_0^{k,p}(\Omega) := \overline{C_0^\infty(\Omega)}^{\|\cdot\|_{W^{k,p}(\Omega)}}$.
- $H^k(\Omega) := W^{k,2}(\Omega)$.
- $\mathbb{R}_+ = (0, \infty)$ and $\mathbb{R}_- = (-\infty, 0)$.
- $\mathbb{R}_+^0 = [0, \infty)$ and $\mathbb{R}_-^0 = (-\infty, 0]$.
- For $R \in \mathbb{R}^+$ we define a ball $B_R(x) = \{y \mid |x - y| < R\}$.
- $\Theta(\alpha, c)$ denotes a sector in the complex plane $\Theta(\alpha, c) = \{z \in \mathbb{C} \mid |\arg(z - c)| \leq \alpha\}$ for $c \in \mathbb{R}$ and $\alpha \in [0, \pi/2)$.
- A continuous embedding of space M into N is denoted as $M(\Omega) \hookrightarrow N(\Omega)$.
- A compact embedding M into N is denoted as $M(\Omega) \hookrightarrow\hookrightarrow N(\Omega)$.

Introduction

Quantum physics is traditionally based on the formulation of several basic postulates. The first says that the state of a system is described by a normalized state vector on a separable Hilbert space. According to the second, each measurable physical quantity is assigned a self-adjoint operator. This was a natural choice, because at the time of the birth of quantum physics, there was already a much stronger mathematical apparatus for them. Now, however, it turns out that such a restriction is too binding and deprives modern physics of many interesting possibilities. However, in order for a theory of non-Hermitian quantum physics to emerge, it is first necessary to introduce a comprehensive mathematical theory for non-self-adjoint operators. Many mathematical physicists are already working on this, and they have already achieved many important results [3] [19] [8].

This thesis is a contribution to this effort. In particular, we focus on matrix-valued operators, which are often simply overlooked. If we consider the energy operator for systems in a magnetic field, we must necessarily include the interaction of the particle spin with the electromagnetic field. This interaction is traditionally represented by Pauli matrices, and due to them we obtain a matrix-valued operator.

In order to talk about Schrödinger operator, we must first introduce it correctly. The Schrödinger operator is an energy operator and therefore consists of kinetic energy, the so-called free Hamiltonian, and potential energy. While a free Hamiltonian is a very well-studied operator that can be easily implemented as a self-adjoint, we cannot say the same about the potential. The traditional definition of observables requiring the self-adjointness of an operator excludes several physical cases, including ordinary complex potential. To correctly introduce the Schrödinger operator as the sum of the kinetic and potential operators, we use unambiguous correspondences of operators and quadratic forms.

We will show that it is appropriate to consider the potentials that are relatively form-bounded with a relative bound less than one. Since it is impractical to verify such a condition for each potential separately, we derive several categories that automatically satisfy it. These conditions are most easily sought in the first and third physical dimensions, which is fortunately consistent with our next course of action. We will also show if and how these conditions change if we consider the magnetic free Hamiltonian instead of the classical one.

Once we introduce the Schrödinger operator, we will focus on studying its spectrum. We determine the spectrum of free Hamiltonian, which is purely essential. We will show that adding local potentials will not change the essential spectrum. Again, we will break down the necessary condition for these potentials in the first and third dimensions.

Once we ensure the stability of the essential spectrum, we can focus on eigenvalues. Without the spectral theorem and other useful properties of self-adjoint operators, it is not easy to explicitly determine the spectrum of the Schrödinger operator. Instead, we will focus on its localization, using the modified

Birman-Schwinger principle. In the first physical dimension, we get an estimate on the eigenvalues. In the third dimension, we show a condition that excludes the existence of eigenvalues altogether.

In total, we will show for what potentials we can well define the Schrödinger operator. Furthermore, we determine the potentials suitable for maintaining the stability of the essential spectrum. Finally, we limit the occurrence of the eigenvalues of the Schrödinger operator to a circle in the complex plane determined by the norm of the potential. For a certain shape of the potential, we will exclude the existence of all eigenvalues and thus obtain an operator with a purely continuous spectrum.

Chapter 1

Motivation

1.1 Quantum physics

Quantum physics is probably the youngest yet fast growing field of physics. Its huge technological impact motivates many mathematicians to explore its limitations. Quantum physics is traditionally defined on infinite-dimensional Hilbert space \mathcal{H} , i.e. a complete vector space with inner product [4]. The state of physical system is described by a wave function, which is a unit vector ψ in the Hilbert space. This corresponds to the probability interpretation of quantum physics. Physical observables are represented by self-adjoint operators A and the measurement outcomes are represented by the spectrum of this operator. In the most common Schrödinger representation the Hilbert space is chosen as

$$L^2(\mathbb{R}^d) := \left\{ \psi : \mathbb{R}^d \rightarrow \mathbb{C} \mid \int_{\mathbb{R}^d} |\psi|^2 < +\infty \right\}.$$

In this representation the time evolution is given by the Schrödinger equation

$$H(t)\psi(\mathbf{r}, t) = i\hbar \frac{\partial \psi(\mathbf{r}, t)}{\partial t}. \quad (1.1)$$

On the right side of this fundamental equation of quantum mechanics we find the time derivative of the wave function multiplied by the imaginary unit i and the reduced Planck constant \hbar . On its left side, the operator of energy H acts on the wave function. However, we will consider only the stationary case and therefore only time-independent Schrödinger operator. This operator is divided into a kinetic energy operator of a quantum particle of mass m , the so-called free Hamiltonian,

$$H_0 = -\frac{\hbar^2}{2m} \Delta, \quad (1.2)$$

and a potential energy operator, denoted as V . The domain of the Schrödinger operator is chosen as a convenient subset of $L^2(\mathbb{R}^d)$, namely

$$D(H_0) = \left\{ \psi \in L^2(\mathbb{R}^d) \mid \Delta\psi \in L^2(\mathbb{R}^d) \right\}, \quad (1.3)$$

and further on, all the wavefunctions will be taken from this subset.

1.2 Self-adjointness

As already mentioned, observables are typically represented by self-adjoint operators. We will show later that introducing a free Hamiltonian as a self-adjoint operator is relatively easy. However, for a potential energy operator, the condition of self-adjointness is not automatic and is often too restrictive for our needs. What is more, there is a growing interest in extending quantum physics to non-self-adjoint operators, which are similar to self-adjoint operators. The growth of this field of physics is slow because many claims about self-adjoint operators and a very strong mathematical apparatus, including the spectral theorem, cannot be used. Nevertheless, there are already many interesting results, as we can see for example in [3]. Our goal will be to extend several of these results to matrix-valued operators and even get new ones.

1.3 Matrix-valued potentials

We have explained our interest in non-self-adjoint operators, so it is time to say why we want to deal with matrix-valued operators. If we include an electromagnetic field, specifically the effect of a particle spin, the Schrödinger equation is no longer enough for us. The non-relativistic quantum equation that explicitly includes this spin is named after the Austrian physicist Wolfgang Pauli and is the compromise between the relativistic Dirac and the already mentioned Schrödinger equation. At first glance, Pauli equation seems the same as Schrödinger equation for vector $\mathbf{r} \in \mathbb{R}^d$ and time $t \in \mathbb{R}$

$$\hat{H}(t)\psi(\mathbf{r}, t) = i\hbar \frac{\partial \psi(\mathbf{r}, t)}{\partial t}. \quad (1.4)$$

The action on wavefunction is determined by the Pauli operator instead of Schrödinger operator

$$\hat{H}\psi = \frac{(-i\hbar\nabla - q\mathbf{A})^2}{2m}\psi + V\psi + \mu\boldsymbol{\sigma}\mathbf{B}\psi. \quad (1.5)$$

The operator includes the charge of the particle q as well as the external electromagnetic field, which is described by magnetic induction \mathbf{B} and electric potential A . These are obtained by solving Maxwell's equations:

$$\begin{aligned} \nabla \cdot \mathbf{A} &= \frac{\rho}{\varepsilon_0}, & \nabla \cdot \mathbf{B} &= 0, \\ \nabla \times \mathbf{A} &= -\frac{\partial \mathbf{B}}{\partial t}, & \nabla \times \mathbf{B} &= \mu_0 \left(\mathbf{J} + \varepsilon_0 \frac{\partial \mathbf{E}}{\partial t} \right). \end{aligned}$$

These equations also introduce the total electric charge density ρ , the electric current density \mathbf{J} and the universal constants ε_0 (the permittivity of free space) and μ_0 (the permeability of free space).

Pauli operator is characteristic mainly by the last component, which represents the interaction of the particle spin with electromagnetic field. It is multiplication of the magnetic induction \mathbf{B} by the magnetic moment μ and Pauli matrices

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \quad (1.6)$$

The Pauli matrix σ , as an observable quantity in quantum mechanics, should satisfy the conditions below. The third condition arises from the fact that the spin behaves as an internal angular momentum and should therefore satisfy the same commutation relations as the orbital angular momentum. These matrices must

- be Hermitian,
- have eigenvalues ± 1 ,
- fulfil commutation relations: $[\sigma_1, \sigma_2] = 2i\hbar\sigma_3$, $[\sigma_2, \sigma_3] = 2i\hbar\sigma_1$, $[\sigma_3, \sigma_1] = 2i\hbar\sigma_2$.

Pauli's matrices are not the only possible solution for these requirements, but they are physically fully equivalent to other solutions. In addition, they are very interesting mathematically. Together with a unit matrix of the appropriate size, they generate all Hermitian matrices 2×2 .

Thus, when including particle spin, there is a need to work with matrix-valued operators. This is a motivation for us to study matrix-valued potentials and their influence on known estimates for Schrödinger potentials.

Chapter 2

Introduction of Schrödinger operators

In this paper we will study the formal definition of the Schrödinger operator with matrix-valued potentials:

$$H_V = -\Delta_{\mathbb{C}^n} + V \quad \text{in} \quad L^2(\mathbb{R}^d, \mathbb{C}^n). \quad (2.1)$$

where matrix-valued function $V : \mathbb{C}^n \rightarrow \mathbb{C}^n$ acts as an operator of multiplication. It is well known how to define such operators in the scalar case (i.e. $n = 1$). We will alter all steps to ensure their validity in higher dimensions. Firstly, it is necessary to define various attributes of operators. Similar attributes will be defined for sesquilinear forms, which we will use in order to define our operator. We will also prove few theorems in order to clarify their relation.

2.1 Definitions

First, we need some definitions and basic theorems, that will be used later. Some of them clearly work for matrix-valued operators, the rest will be altered for purposes of this paper.

Definition 2.1.1. Linear operator A , such that $A : D(A) \rightarrow \mathcal{H}$ is called:

- **densely defined** if $D(A)$ is dense in \mathcal{H} ,
- **closed** if $(\forall \psi \in \mathcal{H}, (\psi_n) \subset D(A) : \psi_n \rightarrow \psi \in \mathcal{H}, A\psi_n \rightarrow \phi \in \mathcal{H}) \Rightarrow (\psi \in D(A) \wedge A\psi = \phi)$,
- **closable** if A has a closed extension $\tilde{A} : D(A) \subset D(\tilde{A}) \wedge \forall \psi \in D(A) : A\psi = \tilde{A}\psi$,
- **symmetric** if it is densely defined and $\forall \phi, \psi \in D(A) : (\psi, A\phi) = (A\psi, \phi)$,
- **bounded** if there exists $M \geq 0$ such that $\|A\psi\| \leq M\|\psi\|$ for all $\psi \in D(A)$; the smallest number with such property is called the norm of operator A ,
- **continuous** if $\forall \psi \in D(A)$ and $\{\psi_n\} \subset D(A)$:

$$\left(D(A) \ni \psi_n \xrightarrow{n \rightarrow \infty} \psi \in \mathcal{H} \wedge A\psi_n \xrightarrow{n \rightarrow \infty} \phi \in \mathcal{H} \right) \Rightarrow (\psi \in D(A)) \wedge A\psi = \phi.$$

Definition 2.1.2. Adjoint operator A^* is defined as

$$D(A^*) := \left\{ \phi \in \mathcal{H} \mid \exists \phi^* \in \mathcal{H}; \forall \psi \in D(A) : (\phi, A\psi) = (\phi^*, \psi) \right\};$$

$$A^* \phi := \phi^*.$$

Operator is called **self-adjoint** if it is densely defined and $A = A^*$.

Definition 2.1.3 (Spectrum). The spectrum of a linear operator A is defined as complement of **resolvent set**

$$\rho(A) := \left\{ z \in \mathbb{C} \mid (A - z) \text{ is injective} \wedge (A - z)^{-1} \in \mathcal{B}(\mathcal{H}) \right\}. \quad (2.2)$$

Definition 2.1.4 (Spectrum of a closed operator). By the closed graph theorem, spectrum of closed linear operator A can be also defined as

$$\sigma(A) := \left\{ \lambda \in \mathbb{C} \mid (A - \lambda) \text{ is not bijective} \right\}. \quad (2.3)$$

Spectrum can be further divided in disjoint sets according to which condition of bijectivity is not fulfilled.

- **point spectrum:** $\sigma_p(A) := \left\{ \lambda \in \mathbb{C} \mid (A - \lambda) \text{ is not injective} \right\} = \left\{ \lambda \in \mathbb{C} \mid \exists \psi \in D(A), \psi \neq 0 : A\psi = \lambda\psi \right\}$,
- **continuous spectrum:** $\sigma_c(A) := \left\{ \lambda \in \sigma(A) \mid (A - \lambda) \text{ is injective} \wedge \overline{\text{Ran}(A - \lambda)} = \mathcal{H} \right\}$,
- **residual spectrum:** $\sigma_r(A) := \left\{ \lambda \in \sigma(A) \mid (A - \lambda) \text{ is injective} \wedge \overline{\text{Ran}(A - \lambda)} \neq \mathcal{H} \right\}$.

For self-adjoint operators A , the spectrum is a subset of real numbers and the residual spectrum is empty.

Definition 2.1.5 (Alternative decomposition of spectrum).

Spectrum can also be divided in disjoint set as

- **discrete spectrum:** $\sigma_{\text{disc}}(H) := \left\{ \lambda \in \sigma_p(H) \mid m(\lambda) = \dim \text{Ker}(H - \lambda) < \infty \wedge \lambda \text{ isolated} \right\}$,
- **essential spectrum:** $\sigma_{\text{ess}}(H) := \left\{ \lambda \in \sigma(H) \setminus \sigma_{\text{disc}}(H) \right\}$.

Definition 2.1.6. We define the *numerical range* of an operator A as:

$$W(A) := \left\{ (A\psi, \psi) \mid \psi \in D(A), \|\psi\| = 1 \right\}. \quad (2.4)$$

Definition 2.1.7. The operator A is called *sectorial*, if $W(A) \subseteq \Theta(\alpha, c)$. The operator called *m-sectorial* if we have again $W(A) \subseteq \Theta(\alpha, c)$, A is closed and $\text{Ran}(A - \alpha I)$ is dense in \mathcal{H} . We call $c \in \mathbb{R}$ a vertex and $\alpha \in [0, \pi/2)$ a corresponding semi-angle.

Remark. The m-sectorial operators are maximal sectorial.

2.2 Sesquilinear forms

Definition 2.2.1. *Sesquilinear form* is a mapping $a : D(a) \times D(a) \rightarrow \mathbb{C}$, where $D(a) \subset \mathcal{H}$, such that

1. $\psi \mapsto a(\phi, \psi)$ is linear for each $\phi \in D(a)$,
2. $\phi \mapsto a(\phi, \psi)$ is semilinear for each $\psi \in D(a)$.

The mapping $a : D(a) \rightarrow \mathbb{C}$ defined as $a[\psi] := a(\psi, \psi)$ is called the *quadratic form associated with a*.

Relation between them is conclusively determined by the *polarisation identity* $\forall \phi, \psi \in D(a)$:

$$a(\phi, \psi) = \frac{1}{4} (a[\phi + \psi] - a[\phi - \psi] + ia[\phi - i\psi] - ia[\phi + i\psi]). \quad (2.5)$$

Many properties can be defined similarly as for operators.

Definition 2.2.2. Quadratic form a is called:

- **densely defined** if $D(a)$ dense in \mathcal{H} ,
- **restriction of \tilde{a}** if $D(a) \subset D(\tilde{a}) \wedge \forall \psi, \phi \in D(a) : a(\psi, \phi) = \tilde{a}(\psi, \phi)$,
- **symmetric** if $a^* = a$,
- **bounded** if there exists $M \geq 0$ such that $a[\psi] \leq M\|\psi\|^2$ for all $\psi \in D(a)$,
- **bounded from below** if there exists $m \in \mathbb{R}$ such that $a[\psi] \geq m\|\psi\|^2$ for all $\psi \in D(a)$.

Definition 2.2.3. *Adjoint form* a^* is defined as

$$\begin{aligned} a^*(\phi, \psi) &:= \overline{a(\psi, \phi)} \\ D(a^*) &:= D(a). \end{aligned}$$

If the symmetric form is bounded from below we simply write $a \geq m$. Symmetric form is called positive if $a \geq 0$. For densely defined, symmetric and bounded from below form we define inner product

$$s_a(\phi, \psi) := a(\phi, \psi) + (1 - m)(\phi, \psi), \quad D(s_a) := D(a), \quad (2.6)$$

where m is in agreement with the definition of a form bounded from below. $(D(a), s_a)$ is a pre-Hilbert space. Form a is said to be *closed* if $(D(a), s_a)$ is complete and *closable* if it has a closed extension. Form a then has the *closure* \bar{a} defined as:

$$D(\bar{a}) := \left\{ \psi \in \mathcal{H} \mid \exists \psi_n \subset D(a) : \psi_n \xrightarrow{n \rightarrow \infty} \psi, a[\psi_n - \psi_m] \xrightarrow{n, m \rightarrow \infty} 0 \right\}, \quad (2.7)$$

$$\bar{a}[\psi] := \lim_{n \rightarrow \infty} a[\psi_n]. \quad (2.8)$$

Definition 2.2.4. We define the *numerical range* of a form a as:

$$W(a) := \{a[\psi] \mid \psi \in D(a), \|\psi\| = 1\}. \quad (2.9)$$

Definition 2.2.5. The form a is called *sectorial*, if $W(a) \subseteq \Theta(\alpha, c)$. We call $c \in \mathbb{R}$ a vertex and $\alpha \in [0, \pi/2)$ a corresponding semi-angle.

2.3 Relation of forms and operators

The easiest way to construct self-adjoint operators is to use one-on-one correspondence between self-adjoint operator A bounded from below and densely defined symmetric closed sesquilinear form a bounded from below. For self-adjoint operator A bounded from below the form is defined as

$$a[\psi] := (\psi, A\psi), \quad D(a) := D(A). \quad (2.10)$$

This form is densely defined, symmetric and bounded from below. Although it is not necessarily closed, it is closable and its closure satisfies all desired properties. The opposite correspondence results from the following theorem:

Theorem 2.3.1 (Representation theorem). *Let a be a densely defined, symmetric, closed form bounded from below in \mathcal{H} . Then the operator*

$$D(A) := \left\{ \psi \in D(a) \mid \exists \eta \in \mathcal{H}, \forall \phi \in D(a), a(\phi, \psi) = (\phi, \eta) \right\},$$

$$A\psi := \eta,$$

is self-adjoint and bounded from below.

This is consequence of Riesz theorem [17]. Following (2.10), the norm corresponding to free Hamiltonian is defined as

$$h_0[\psi] := (\psi, H_0\psi) = \int_{\mathbb{R}^d} |\nabla\psi|^2. \quad (2.11)$$

Claim 2.3.1. *Form h_0 is densely defined, symmetric, closed and bounded from below.*

Proof. 1. First we prove it for the scalar case.

- Symmetry and boundedness from below is obvious since $\forall \psi \in \text{Dom } h_0 : h_0[\psi] \in \mathbb{R}$ and $h_0[\psi] \geq 0$.
- Form is densely defined because $C_0^\infty(\mathbb{R}^d) \subset \text{Dom } h_0 \wedge \overline{C_0^\infty(\mathbb{R}^d)} = L^2(\mathbb{R}^d)$
- To prove the form is closed, we need $(\forall \psi \in L^2(\mathbb{R}^d), \psi_m \in H^1(\mathbb{R}^d)) :$

$$\left(\|\psi_m - \psi\| \xrightarrow{m \rightarrow \infty} 0 \wedge \|\nabla\psi_m - \nabla\psi\| \xrightarrow{m, p \rightarrow \infty} 0 \right) \Rightarrow \left(\psi \in W^{1,2}(\mathbb{R}^d) \wedge \|\nabla\psi_m - \nabla\psi\| \xrightarrow{m \rightarrow \infty} 0 \right).$$

From closedness of L^2 we know, that $\exists g \in L^2(\mathbb{R}^d, \mathbb{C}^d) : \|\nabla\psi_m - g\| \xrightarrow{m \rightarrow \infty} 0$. So for all test functions $\varphi \in C_0^\infty(\mathbb{R}^d) : (-\nabla\varphi, \psi) = \lim_{m \rightarrow \infty} (-\nabla\varphi, \psi_m) = \lim_{m \rightarrow \infty} (\varphi, \nabla\psi_m) = (\varphi, g)$, therefore $\psi \in W^{1,2}(\mathbb{R}^d) \wedge \nabla\psi = g$.

2. The first three properties can be proved for matrix case by using the same arguments. The proof of the last claim is also quite similar, the process is applied in each component of the function ψ . In n -th second spinor dimension we have

$$h_0[\psi] = \int_{\mathbb{R}^d} \sum_{i=1}^n |\nabla\psi_i|^2 = \|\nabla\psi\|^2$$

for $\psi \in L^2(\mathbb{R}^d, \mathbb{C}^n)$. Similarly to the previous point, we need to show, that $\forall \psi \in L^2(\mathbb{R}^d, \mathbb{C}^n)$ and $\{\psi_m\} \subset H^1(\mathbb{R}^d, \mathbb{C}^n)$:

$$\left(\|\psi_m - \psi\| \xrightarrow{m \rightarrow \infty} 0 \wedge \|\nabla \psi_m - \nabla \psi\| \xrightarrow{m, p \rightarrow \infty} 0 \right) \Rightarrow \left(\psi \in H^1(\mathbb{R}^d, \mathbb{C}^2) \wedge \|\nabla \psi_m - \nabla \psi\| \xrightarrow{m \rightarrow \infty} 0 \right).$$

All of these convergences are in $L^2(\mathbb{R}^d, \mathbb{C}^n)$ and relevant norms are defined as

$$\|\psi\|_{L^2(\mathbb{R}^d, \mathbb{C}^n)} := \left(\int_{\mathbb{R}^d} \sum_{i=0}^n |\psi_i|^2 \right)^{\frac{1}{2}}.$$

Therefore we just replicate the previous process for an arbitrary test function $\varphi \in C_0^\infty(\mathbb{R}^d)$ and each component of the function:

$$\begin{aligned} (-\nabla \varphi, \psi_1) &= \dots = (\varphi, g_1) \\ (-\nabla \varphi, \psi_2) &= \dots = (\varphi, g_2) \\ &\vdots \\ (-\nabla \varphi, \psi_n) &= \dots = (\varphi, g_n). \end{aligned}$$

Clearly $(\nabla \psi)_i = (g)_i$ for all $i = 1 \dots n$. Therefore $\nabla \psi = g \in L^2(\mathbb{R}^d, \mathbb{C}^n)$ and $\psi \in H^1(\mathbb{R}^d, \mathbb{C}^n)$. □

The quadratic form defined as (2.11) satisfies conditions of Representation Theorem 2.3.1 and therefore corresponds with self-adjoint and bounded from below operator H_0 . This formulation is unnecessarily restrictive for our purposes because we do not expect to obtain a self-adjoint operator. It is therefore enough for us to work with sectorial operators.

Theorem 2.3.2 (Representation theorem for sectorial forms). *Suppose that a is a densely defined closed sectorial form on \mathcal{H} . Then we have:*

- (i) *The associated operator A is m -sectorial*
- (ii) *$D(A)$ is a dense linear subspace of the Hilbert space $(D(a), \|\cdot\|_{Re a})$.*

When we have well-defined individual operators H and V , we deal with what happens when we add them together. It is obvious that operators do not have to retain all the properties, so it is necessary to impose additional conditions.

Definition 2.3.1 (Relative boundedness). *Let a be symmetric and bounded from below in \mathcal{H} . A form b is said to be relatively bounded with respect to a if*

- (i) $D(a) \subset D(b)$
- (ii) $\exists \alpha, \beta \geq 0, \forall \psi \in D(a) : |b[\psi]| \leq \alpha a[\psi] + \beta \|\psi\|^2$.

The lowest constant α meeting inequality in the second condition is called the *relative bound* of b with respect to a .

This condition is used to ensure the stability of closedness. If we needed the sum of forms to satisfy the conditions of Theorem (2.3.1), the following theorem would ensure that.

Theorem 2.3.3 (Stability of closedness). *Let a be symmetric, closed and bounded from below in \mathcal{H} . Let b be symmetric and relatively bounded with respect to a with the relative bound less than one. Then the form c defined as*

$$\begin{aligned} c &:= a + b \\ D(c) &:= D(a + b) = D(a) \cap D(b) = D(a) \end{aligned}$$

is symmetric, closed and bounded from below.

However, since we want to use Theorem 2.3.2 instead of Theorem 2.3.1, it is enough to obtain a sectorial form instead of a symmetric one.

Theorem 2.3.4 (Stability of closedness for sectorial forms). *Let a be a sectorial form and let b be relatively bounded with respect to a with the relative bound less than one. Then $c := a + b$ is sectorial. The form c is closed if and only if a is closed, it is closable if and only if a is closable and $D(c) = D(a) \cap D(b)$*

Proof can be found in [17]. Combining this result with the representation Theorem 2.3.2 and substituting $a = h_o, b = v$ results in following theorem. Its general self-adjoint formulation is called Kato-Lions-Lax-Milgram-Nelson theorem [22].

Theorem 2.3.5. *Let H_0 be a self-adjoint operator bounded from below in \mathcal{H} and h_0 the associated sesquilinear form. Let v be a form relatively bounded with respect to h_0 with the relative bound less than one. Then the operator H_V associated with the form $h_V = h_0 + v$ is m -sectorial and $D(H_0)$ is a dense linear subspace of the Hilbert space $(D(h_0), \|\cdot\|_{Re h_0})$.*

Remark (Notation). This theorem allows us to properly introduce the sum of the operators, using the associated forms. Introduction through forms is traditionally indicated by writing a dot above the plus in the expression $H_V = H_0 \dot{+} V$.

Chapter 3

Relatively form-bounded perturbations with respect to free Hamiltonian

In this chapter we will focus on the potential operator and the conditions on it. It follows from Theorem 2.3.5 that we need the form corresponding to the operator V to be relatively bounded with respect to the form of a free Hamiltonian with a relative bound less than one. Let us consider a potential $V : \mathbb{C}^n \rightarrow \mathbb{C}^n$. Its corresponding quadratic form can be defined as $v[\psi] = \int_{\mathbb{R}^d} \psi^* V \psi$ for every $\psi \in C_0^\infty(\mathbb{R}^d, \mathbb{C}^n)$. Specifically, we have

$$v[\psi] = \int_{\mathbb{R}^d} \left(\sum_{j,k=1}^n \overline{\psi_j} V_{jk} \psi_k \right) dx, \quad (3.1)$$

where $V_{jk} \in L_{\text{loc}}^1(\mathbb{C}^n)$ for all $j, k = 1, \dots, n$. From Theorem 2.3.5 immediately follows that in order for Schrödinger operator to be closed, the condition of relative boundedness to free Hamiltonian must be met. We require

$$|v[\psi]| \leq \alpha h_0[\psi] + \beta \|\psi\|^2, \quad (3.2)$$

where α must be less than one. Since this condition is unpleasant for verification in each individual case, we derive sufficient conditions for potentials from known inequalities and relations. Obviously,

$$|v[\psi]| \leq \int_{\mathbb{R}^d} |V(x)|_{\mathbb{C}^n} |\psi(x)|_{\mathbb{C}^n}^2 dx, \quad (3.3)$$

which makes the process similar to the scalar case and that will be used in further procedures.

3.1 Hardy inequality

In the dimension $d \geq 3$, the following Hardy inequality holds for the free Hamiltonian

$$h_0[\psi] \geq \left(\frac{d-2}{2} \right)^2 \int_{\mathbb{R}^d} \frac{|\psi|^2}{|x|^2}. \quad (3.4)$$

By combining the estimate (3.3) and (3.4) and adding it to the condition (3.2), we get

$$\begin{aligned} |v[\psi]| &\leq \int_{\mathbb{R}^d} |V(x)|_{\mathbb{C}^n} |\psi(x)|_{\mathbb{C}^n}^2 dx \\ &\leq \alpha \left(\frac{d-2}{2} \right)^2 \int_{\mathbb{R}^d} \frac{|\psi(x)|_{\mathbb{C}^n}^2}{|x|^2} dx + \beta \int_{\mathbb{R}^d} |\psi(x)|_{\mathbb{C}^n}^2 dx \\ &\leq \alpha h_0[\psi] + \beta \|\psi\|^2 \end{aligned}$$

From here we easily obtain the condition for the matrix norm of the potential function

$$|V(x)|_{\mathbb{C}^n} \leq \alpha \left(\frac{d-2}{2} \right)^2 \frac{1}{|x|^2} + \beta \quad \text{with} \quad \alpha < 1. \quad (3.5)$$

3.2 Sobolev inequality

In the third and higher dimensions we can also use one particular Sobolev inequality to derive the condition on potential, namely,

$$\int_{\mathbb{R}^d} |\nabla \psi|^2 \geq C_d \left(\int_{\mathbb{R}^d} |\psi|^{f^*(d)} \right)^{\frac{2}{f^*(d)}}, \quad (3.6)$$

where

$$C_d = \frac{d(d-2)|S_d|^{\frac{2}{d}}}{4} \quad (3.7)$$

is a fixed constant dependent on dimension and $f^*(d)$ is a function defined as

$$f^*(d) = \frac{2d}{d-2}. \quad (3.8)$$

Now we estimate the potential form.

$$\begin{aligned} |v[\psi]| &\leq \int_{\mathbb{R}^3} |V(x)|_{\mathbb{C}^n} |\psi(x)|_{\mathbb{C}^n}^2 dx \\ &\leq \left(\int_{\mathbb{R}^3} |V(x)|_{\mathbb{C}^n}^p \right)^{\frac{1}{p}} \left(\int_{\mathbb{R}^3} |\psi|_{\mathbb{C}^n}^{2q} \right)^{\frac{1}{q}} \\ &\leq \| |V(x)|_{\mathbb{C}^n} \|_{L^p} \|\psi\|_{L^{2q}}^2. \end{aligned}$$

We used Hölder inequality

$$\int |fg| \leq \left(\int |f|^p \right)^{\frac{1}{p}} \left(\int |g|^q \right)^{\frac{1}{q}} \quad \text{where} \quad \frac{1}{p} + \frac{1}{q} = 1. \quad (3.9)$$

Now we use Sobolev inequality (3.6) as

$$\|\psi\|_{L^{f^*(d)}}^2 \leq \frac{1}{C_d} h_0[\psi]. \quad (3.10)$$

We set

$$q = \frac{f^*(d)}{2} \quad \text{and} \quad p = \frac{f^*(d)}{f^*(d) - 2} = \frac{d(d-2)}{2} \quad (3.11)$$

and we connect the expressions as

$$|v[\psi]| \leq \| |V(x)|_{\mathbb{C}^n} \|_{L^{\frac{d(d-2)}{2}}} \|\psi\|_{L^{f^*(d)}}^2 \leq |V(x)|_{\mathbb{C}^n} \|_{L^{\frac{d(d-2)}{2}}} \frac{1}{C_d} h_0[\psi].$$

In order to make the last estimation less than $\alpha h_0[\psi]$, potential must fulfil

$$\| |V(x)|_{\mathbb{C}^n} \|_{L^{\frac{d(d-2)}{2}}} \leq \alpha C_d < C_d. \quad (3.12)$$

3.3 First dimension

If the dimension d is equal to one, we estimate the integral as

$$\begin{aligned} \int_{\mathbb{R}} |V(x)|_{\mathbb{C}^n} |\psi(x)|_{\mathbb{C}^n}^2 dx &= \int_{\mathbb{R}} \left(\frac{d}{dx} \int_{-\infty}^x |V(\xi)|_{\mathbb{C}^n} d\xi \right) |\psi(x)|^2 dx \\ &= - \int_{\mathbb{R}} \left(\int_{-\infty}^x |V(\xi)|_{\mathbb{C}^n} d\xi \right) 2|\psi(x)| |\psi'(x)| dx \\ &\leq \| |V(x)|_{\mathbb{C}^n} \|_{L^1} 2\|\psi\| \|\psi'\| \\ &\leq \varepsilon \|\psi'\|^2 + \frac{1}{\varepsilon} \|V\|_{L^1}^2 \|\psi\|^2. \end{aligned}$$

Here we used Young's inequality

$$ab \leq \frac{a^2}{2\varepsilon} + \frac{\varepsilon b^2}{2} \quad (3.13)$$

for all $\varepsilon > 0$. We simply choose $\alpha = \varepsilon < 1$ and $\beta = \frac{1}{\varepsilon} \| |V(x)|_{\mathbb{C}^n} \|_{L^1}^2$ and the condition (3.2) will be met. It is of course necessary for potential V to be in $L^1(\mathbb{R})$.

3.4 Kato class

Another group of potentials that meet the condition (3.2) are functions from the Kato class.

Definition 3.4.1 (Kato class of order a). For all $a > 0$ we say potential $V \in K_a(\mathbb{R}^d)$ if

$$\begin{aligned} \sup_{x \in \mathbb{R}^d} \int_{|x-y| < 1} |V(y)| dy &< \infty && \text{for } a > d, \\ \lim_{\delta \rightarrow 0} \sup_{x \in \mathbb{R}^d} \int_{|x-y| < \delta} w_a(x-y) |V(y)| dy &= 0 && \text{for } 0 < a \leq d, \end{aligned}$$

where

$$w_a(x) := \begin{cases} |x|^{a-d} & \text{for } 0 < a < d, \\ \ln|x|^{-1} & \text{for } a = d \\ 1 & \text{for } a > d. \end{cases}$$

Definition 3.4.2 (Kato class). We say that potential V is in *Kato class* ($V \in \mathcal{K}(\mathbb{R}^d)$) if it satisfies the previous definition for $a = 2$.

The Kato potentials satisfy the condition of relative boundedness with respect to h_0 , as shown, for example, in [26]. Therefore, it is another potential class suitable for the correct definition of the Schrödinger operator.

Using the obtained estimates, we can propose the following summary criterion.

Proposition 3.4.1. *Let us consider a free Hamiltonian defined on $H^1(\mathbb{R}^d, \mathbb{C}^n)$. If the potential function $V : \mathbb{C}^n \rightarrow \mathbb{C}^n$ acting as an operator with associated form v defined as (3.1) meets one of the following conditions:*

- $|V(x)|_{\mathbb{C}^n} \leq \alpha \left(\frac{d-2}{2}\right)^2 \frac{1}{|x|^2} + \beta$ with $\alpha < 1$ for $d \geq 3$,
- $\| |V(x)|_{\mathbb{C}^n} \|_{L^{\frac{d(d-2)}{2}}(\mathbb{R}^d)} < C_d$ for $d \geq 3$,
- $V \in L^1(\mathbb{R})$ for $d = 1$,
- $V \in \mathcal{K}(\mathbb{R}^d)$ for $d \geq 1$,

then form v is relatively bounded with respect to h_0 with relative bound less than one.

By combining this proposition with the stability of closedness (2.3.4) and altered KLMN Theorem 2.3.5, we find that h_V defined as $h_V = h_0 + v$ is closed. Operator $H_V = H_0 + V$ is closed and m -sectorial. Moreover, if the potential function $V(x)$ is Hermitian for almost every $x \in \mathbb{R}^d$, the corresponding operator is also self-adjoint.

From here, it is obvious that the easiest way to introduce an operator is to use the conditions for potential in the first and third dimensions. This might seem insufficient, but we know from practice that these two dimensions are the most physically significant. Later, we will come across other conditions, due to which we limit ourselves to these two dimensions.

Chapter 4

Condition for magnetic Hamiltonian

All the above conditions are derived from the form of the free Hamiltonian in the Schrödinger operator. However, the Pauli operator (1.5) differs not only by potential involving the interaction of the electromagnetic field but also by the free Hamiltonian itself. In agreement with kinetic momenta in classical physics, the free magnetic Hamiltonian is introduced via:

$$H_A = (-i\nabla - \mathbf{A})^2 \quad (4.1)$$

with associated sesquilinear form

$$h_A[\psi] = \int_{\mathbb{R}^d} |-i\nabla\psi - \mathbf{A}\psi|^2 dx \geq 0 \quad (4.2)$$

defined on magnetic Sobolev space

$$D(h_A) = H_A^1(\mathbb{R}^d) = \overline{C_0^\infty(\mathbb{R}^d)}^{\|\cdot\|_A}, \quad (4.3)$$

where $\|\cdot\|_A = \sqrt{h_A[\cdot] + \|\cdot\|^2}$.

Free magnetic Hamiltonian is obviously different from the classical, so it is not possible to use the results from the previous chapter without further modifications. Fortunately, the following diamagnetic inequality [20] saves us a lot of trouble.

Theorem 4.0.1 (Diamagnetic inequality). *Let $\mathbf{A} : \mathbb{R}^d \rightarrow \mathbb{R}^d$ be in $L_{loc}^2(\mathbb{R}^d)$ and let ψ be in $H_A^1(\mathbb{R}^d)$. Then $|\psi| \in H_A^1(\mathbb{R}^d)$ and the diamagnetic inequality*

$$|(-i\nabla - \mathbf{A})\psi(x)| \geq |\nabla|\psi|(x)|. \quad (4.4)$$

holds pointwise for almost every $x \in \mathbb{R}^d$.

Using this relation, we can rewrite some of the conditions from the previous chapter.

4.1 Condition on potentials

The goal is to make potential relatively bounded to free magnetic Hamiltonian h_A with relative bound α less than one:

$$|v[\psi]| \leq \alpha h_A[\psi] + \beta \|\psi\|^2. \quad (4.5)$$

From the form of the Pauli operator (1.5), it is obvious that in this case it is especially important that the procedure also works for matrix-valued potentials. This is once again made possible by an estimate

$$|v[\psi]| \leq \int_{\mathbb{R}^d} |V(x)|_{\mathbb{C}^n} |\psi(x)|^2 dx. \quad (4.6)$$

This estimation converts a complex matrix-valued function $V(x) : \mathbb{C}^n \rightarrow \mathbb{C}^n$ into a scalar and real form $|V(x)|_{\mathbb{C}^n} : \mathbb{C}^n \rightarrow \mathbb{R}$. This simplification is only possible due to the shape of condition (4.5) and again requires that the potential satisfies $V_{j,k} \in L^1_{\text{loc}}(\mathbb{R}^d)$. All of the following procedures are performed for functions $\psi \in H^1_A(\mathbb{R}^d, \mathbb{C}^n)$ and that correspond to the norms used (i.e. $\|\cdot\|_{L^2} = \|\cdot\|_{L^2(\mathbb{R}^d, \mathbb{C}^n)}$).

4.1.1 Hardy inequality

For dimension $d \geq 3$:

$$h_0[\psi] \geq \left(\frac{d-2}{2}\right)^2 \int \frac{|\psi|^2}{|x|^2}. \quad (4.7)$$

By rewriting the condition in terms of norms, we obtain:

$$\|\nabla\psi\|_{L^2}^2 \geq \left(\frac{d-2}{2}\right)^2 \left\| \frac{\psi}{|x|} \right\|_{L^2}^2. \quad (4.8)$$

This also stands for positive function $|\psi|$, which allows us to use diamagnetic inequality (4.4):

$$h_A[\psi] = \|(-i\nabla - A)\psi\|_{L^2}^2 \geq \|\nabla|\psi|\|_{L^2}^2 \geq \left(\frac{d-2}{2}\right)^2 \left\| \frac{|\psi|}{|x|} \right\|_{L^2}^2 = \left(\frac{d-2}{2}\right)^2 \left\| \frac{\psi}{|x|} \right\|_{L^2}^2. \quad (4.9)$$

It is clear from this estimate that we obtain the same potential condition as in the previous chapter:

$$|V(x)|_{\mathbb{C}^n} \leq \alpha \left(\frac{d-2}{2}\right)^2 \frac{1}{|x|^2} + \beta \quad \text{with} \quad \alpha < 1. \quad (4.10)$$

4.1.2 Sobolev inequality

Again, we start from this Sobolev inequality for free Hamiltonian

$$\int_{\mathbb{R}^d} |\nabla\psi|^2 \geq C \left(\int |\psi|^{f^*(d)} \right)^{\frac{1}{f^*(d)}}, \quad (4.11)$$

where

$$C_d = \frac{d(d-2)|S_d|^{\frac{2}{d}}}{4} \quad (4.12)$$

is a fixed constant dependent on dimension and $f^*(d)$ is a function defined as $f^*(d) = \frac{d-2}{2d}$. We once again rewrite it using forms:

$$\|\nabla\psi\|_{L^2} \geq C \|\psi\|_{L^{f^*(d)}}. \quad (4.13)$$

Now thanks to diamagnetic inequality we receive very similar estimate:

$$h_A[\psi] \geq h_0[\psi] \geq C \|\psi\|_{L^{f^*(d)}} = C \|\psi\|_{L^{f^*(d)}}. \quad (4.14)$$

This means that we can adapt the estimate from the last chapter:

$$\int_{\mathbb{R}^3} |V(x)|_{\mathbb{C}^n} |\psi(x)|_{\mathbb{C}^n}^2 dx \leq \| |V(x)|_{\mathbb{C}^n} \|_{L^{\frac{3}{2}}} \|\psi\|_{L^6}^2 \leq \| |V(x)|_{\mathbb{C}^n} \|_{L^{\frac{3}{2}}} \frac{1}{C_d} h_A[\psi].$$

In order for the last estimate to be less than $\alpha h_A[\psi]$, the potential must fulfil

$$\| |V(x)|_{\mathbb{C}^n} \|_{L^{\frac{d(d-2)}{2}}} \leq \alpha C_d < C_d. \quad (4.15)$$

4.1.3 First dimension

In the first dimension and on the real axis we have the so-called gauge invariance. That means the free Hamiltonian in magnetic field is unitarily equivalent to the classical free Hamiltonian. Should we want to proceed with the magnetic field anyway, the process could easily be altered because

$$\begin{aligned} \int_{\mathbb{R}} \left(|\psi(x)|^2 \right)' dx &= \int_{\mathbb{R}} 2 \operatorname{Re} \left(\overline{\psi(x)'} \psi(x) \right) dx \\ &\leq 2 \left(\int_{\mathbb{R}} |\psi(x)'|^2 dx \right)^{\frac{1}{2}} \left(\int_{\mathbb{R}} |\psi(x)|^2 dx \right)^{\frac{1}{2}} \\ &\leq 2 \left(\int_{\mathbb{R}} |\psi(x)' - iA|^2 dx \right)^{\frac{1}{2}} \left(\int_{\mathbb{R}} |\psi(x)|^2 dx \right)^{\frac{1}{2}}. \end{aligned}$$

By a procedure analogous to that of the previous chapter, we obtain

$$\int_{\mathbb{R}} |V(x)| |\psi(x)|^2 dx \leq \varepsilon h_A[\psi] + \frac{1}{\varepsilon} \|V\|_{L^1}^2 \|\psi\|^2. \quad (4.16)$$

That holds for all $\varepsilon > 0$. We simply choose $\alpha = \varepsilon < 1$ and $\beta = \frac{1}{\varepsilon} \|V\|_{L^1}^2$ if $V \in L^1$ and the condition (4.5) will be met.

Using the obtained estimates, we can propose the following criterion similarly as (3.4.1).

Proposition 4.1.1. *Let us consider a free magnetic Hamiltonian defined on $H_A^1(\mathbb{R}^d, \mathbb{C}^n)$. If the potential function $V : \mathbb{C}^n \rightarrow \mathbb{C}^n$ acting as an operator with associated form v defined as (3.1) meets one of the following conditions:*

- $|V(x)|_{\mathbb{C}^n} \leq \alpha \left(\frac{d-2}{2}\right)^2 \frac{1}{|x|^2} + \beta$ with $\alpha < 1$ for $d \geq 3$,
- $\| |V(x)|_{\mathbb{C}^n} \|_{L^{\frac{d(d-2)}{2}}} < C_d$ for $d \geq 3$,
- $V \in L^1(\mathbb{R})$ for $d = 1$,

then form v is relatively bounded with respect to h_A with relative bound less than one.

By combining this proposition with the stability of closedness (2.3.4) and altered KLMN Theorem 2.3.5, we find that h_V defined as $h_V = h_A + v$ is closed. Corresponding operator $H_V = H_A + V$ is also closed and m -sectorial. This operator will be self-adjoint if the potential function $V(x)$ is Hermitian for almost every $x \in \mathbb{R}^d$.

Chapter 5

Stability of the essential spectrum

Once we have a well-defined operator, it is time to study its properties. Specifically, we focus on the spectrum, which in quantum physics represents the possible outcomes of measurements. Since we have no guarantee of the self-adjointness of the energy operator, we cannot rely on many useful tools such as the spectral theorem. Others have dealt with the topic of non-self-adjoint operators and their spectrum before us and obtained useful results [18] [19]. Some of them focus on the essential spectrum and its stability. Our goal is to focus on those potentials whose addition to the free Hamiltonian does not change its essential spectrum. This will allow us later to focus exclusively on the point spectrum and its localization.

5.1 Spectrum of the free Hamiltonian

In order to discuss in which cases the essential spectrum remains unchanged after the addition of the potential, it is first necessary to determine this spectrum. So let's start with the spectrum of the free Hamiltonian. First, we will make a few statements, their proofs can be found, for example, in [4].

Theorem 5.1.1 (Weyl's criterion). *Let A be a self-adjoint operator in \mathcal{H} . One has $\lambda \in \sigma(A) \Leftrightarrow \exists \{\psi_m\} \subset D(A)$ such that:*

1. $\|\psi_m\| = 1$,
2. $\|(A - \lambda)\psi_m\| \xrightarrow{m \rightarrow +\infty} 0$.

Moreover if it in addition to points 1) and 2) also holds that $\psi_m \xrightarrow{m \rightarrow \infty} 0$ in \mathcal{H} , then $\lambda \in \sigma_{\text{ess}}(A)$.

Theorem 5.1.2 (Minimax principle). *Let A be self-adjoint in \mathcal{H} that is bounded from below. We define a non-decreasing sequence $\{\lambda_m\}_{m=1}^{+\infty}$ as*

$$\lambda_m := \inf_{S^m \subset D(A)} \sup_{\psi \in S^m} \frac{(\psi, A\psi)}{\|\psi\|^2}, \quad (5.1)$$

where \mathcal{S}^m is an arbitrary m -dimensional subspace of the corresponding domain and

$$\lambda_\infty := \lim_{m \rightarrow +\infty} \lambda_m. \quad (5.2)$$

Then

1. $\lambda_\infty = \inf \sigma_{\text{ess}}(A)$,
2. $\{\lambda_m\}_{m=1}^\infty \cap (-\infty, \lambda_\infty) = \sigma_{\text{disc}}(A) \cap (-\infty, \lambda_\infty)$.

It is traditionally defined that $\sigma_{\text{ess}}(A) = \emptyset$ if $\lambda_\infty = +\infty$ [4]. This theorem allows us to easily find the lower threshold of the spectrum.

Theorem 5.1.3 (Consequences of the Minimax principle). *Using the same notation*

1. $\inf \sigma(A) = \inf_{\substack{\psi \in D(A) \\ \psi \neq 0}} \frac{(\psi, A\psi)}{\|\psi\|^2}$,
2. $\forall \psi \in D(A) : \inf \sigma(A) \leq \frac{(\psi, A\psi)}{\|\psi\|^2}$,
3. $A_1 \leq A_2 \Rightarrow \lambda_n(A_1) \leq \lambda_n(A_2)$.

Where the last statement holds in terms of associated quadratic forms. Finally, we come to the very spectrum of free Hamiltonian.

Theorem 5.1.4 (Spectrum of free Hamiltonian). *The spectrum of free Hamiltonian is purely essential and equals the non-negative real half-axis : $\sigma(H_0) = \sigma_c(H_0) = [0, +\infty)$.*

Proof. Proof of this theorem will be divided in three parts. For simplicity, the proof is given only for the scalar case. However, since the matrix-valued free Hamiltonian is only a multiplication of the scalar operator and the unit matrix, it is sufficient to repeat the following procedure for each component, similarly as in the proof of Claim 2.3.1.

1. $\sigma(H_0) = \sigma_c(H_0)$

In order to find eigenvalues we solve $-\Delta\psi = \lambda\psi$. Solutions of this equation are given as superpositions of functions e^{ikx} , where $k^2 = \lambda$, $k \in \mathbb{C}^d$. However none of these functions can be eigenfunctions of free Hamiltonian as they do not belong in its domain. This suggests that the spectrum must be purely continuous. To prove it, one conventionally uses the Fourier transform. Alternatively, one can use the method of multipliers [6].

2. $\sigma(H_0) \subset [0, +\infty)$

From (5.1.3) we know that $\inf \sigma(H_0) = \inf_{\substack{\psi \in D(H_0) \\ \psi \neq 0}} \frac{(\psi, H_0\psi)}{\|\psi\|^2}$ and concurrently H_0 is a positive operator

because $(\psi, H_0\psi) = \|\nabla\psi\|^2 \geq 0$. Altogether we receive $\inf \sigma(H_0) \geq 0$.

3. $\sigma(H_0) \supset [0, +\infty)$

We use Weyl's criterion (5.1.1) to prove this inclusion. Because classical solution - as seen in the first part of this proof - are bounded, we can approximate them for $\lambda := k^2$, $k \in \mathbb{R}^d$ and $n \in \mathbb{N}$

$$\psi_n(x) := \varphi_n(x) e^{ikx},$$

where

$$\varphi_n(x) := N_n \varphi\left(\frac{x}{n}\right)$$

with normalising prefactor $N_n = n^{-\frac{d}{2}}$. Function $\varphi \in C_0^\infty(\mathbb{R}^d)$ is normalised to 1 in $L^2(\mathbb{R}^d)$. From this $\forall n \in \mathbb{N}$ we have

$$\|\varphi_n\| = 1, \quad \|\nabla\varphi_n\| = \frac{\|\nabla\varphi\|}{n}, \quad \|\Delta\varphi_n\| = \frac{\|\Delta\varphi\|}{n^2}. \quad (5.3)$$

Every function from sequence (ψ_n) belongs to $C_0^\infty(\mathbb{R}^d) \subset D(H_0)$. We also receive the following relations, which prove useful for working with said sequence:

$$\begin{aligned} \psi_n &:= e^{ikx} \varphi_n(x), \\ \nabla\psi_n &= \nabla\varphi_n e^{ikx} + ik\varphi_n e^{ikx}, \\ \Delta\psi_n &= (\Delta\varphi_n + 2ik\nabla\varphi_n - k^2\varphi_n) e^{ikx}. \end{aligned}$$

Now we apply the operator $(H - k^2)$ in order to verify second statement from (5.1.1):

$$\begin{aligned} \|(H - k^2)\psi_n\| &= \|-\Delta\psi_n - k^2\psi_n\| \\ &= \|(e^{ikx})(2ik\nabla\varphi_n + \Delta\varphi_n)\| \\ &= \|\Delta\varphi_n + 2ik\nabla\varphi_n\| \\ &\leq \|\Delta\varphi_n\| + 2|k|\|\nabla\varphi_n\|. \end{aligned}$$

Using (5.3) we obtain

$$\|(H - k^2)\psi_n\| \xrightarrow{n \rightarrow +\infty} 0.$$

and by applying Weyl's criterion for $(\forall k \in \mathbb{R})(k^2 \in \sigma(H_0))$ we receive $\sigma(H_0) \supset [0, +\infty)$.

□

5.2 Potentials vanishing in infinity

It is quite common that the Schrödinger operator is obtained from free Hamiltonian only by adding a "small" perturbation. One way to ensure the stability of the essential spectrum after the addition of a potential is to demand a condition on the "smallness" of the potential function in the sense that the essential spectrum is not changed. If the potential disappears at infinity, the following theorem applies.

Theorem 5.2.1 (Stability of essential spectrum). *Let $H = H_0 + V$ self-adjoint operator, where bounded potential V suffices*

$$\lim_{R \rightarrow \infty} \|V\|_{L^\infty(\mathbb{R}^d \setminus B_R(0))} = 0,$$

then $\sigma_{\text{ess}}(H) = \sigma(H_0) = [0, +\infty)$.

Proof. We will divide the proof in two sections.

1. $\sigma_{\text{ess}}(H) \supset [0, +\infty)$

Restriction on potential V allows us to use the corresponding part of proof of Theorem 5.1.4 similarly.

2. $\sigma_{\text{ess}}(H) \subset [0, +\infty)$

It is clear that $\sigma_{\text{ess}}(H) \subset [0, +\infty) \Leftrightarrow \min \sigma_{\text{ess}}(H) \geq 0$. For the associated form h

$$H \xleftrightarrow{1-1} h[\psi] = (\psi, H\psi) = \int_{\mathbb{R}^d} |\nabla\psi|^2 + \int_{\mathbb{R}^d} \bar{\psi}V\psi \, dx. \quad (5.4)$$

We further divide the space in restricted (interval $(-L, L)^d$) and unrestricted ($\mathbb{R}^d \setminus (-L, L)^d := I_{\text{ext}}$) compound and on them we define operators with Neumann boundary conditions H_{int}^N and H_{ext}^N . For operators and their associated forms:

$$H \geq H^N = H_{\text{int}}^N \oplus H_{\text{ext}}^N \quad \text{and} \quad h[\psi] \geq h^N[\psi] = h_{\text{int}}^N[\psi] + h_{\text{ext}}^N[\psi]. \quad (5.5)$$

Now we estimate the minimum of $\sigma_{\text{ess}}(H)$ from below with expression converging to zero.

$$\begin{aligned} \min \sigma_{\text{ess}}(H) &\geq \min \sigma_{\text{ess}}(H^N) \\ &= \min \left\{ \min \sigma_{\text{ess}}(H_{\text{ext}}^N), \underbrace{\min \sigma_{\text{ess}}(H_{\text{int}}^N)}_{\emptyset} \right\} \\ &= \min \sigma_{\text{ess}}(H_{\text{ext}}^N) \\ &\geq \min \sigma(H_{\text{ext}}^N) \\ &\geq -\|V\|_{L^\infty(I_{\text{ext}})} \xrightarrow{|L| \rightarrow +\infty} 0. \end{aligned}$$

Here we used the fact that

$$\begin{aligned} h_{\text{ext}}^N[\psi] &= \int_{I_{\text{ext}}} |\nabla\psi|^2 + \int_{I_{\text{ext}}} \bar{\psi}V\psi \geq \int_{I_{\text{ext}}} \bar{\psi}V\psi \\ &\geq -\|V\|_{L^\infty(I_{\text{ext}})} \|\psi\|_{L^2(I_{\text{ext}})}^2. \end{aligned}$$

Altogether we receive $\min \sigma_{\text{ess}}(H) \geq 0$.

□

Moreover, if the potential is non-negative, the resulting spectrum will be purely essential.

Theorem 5.2.2. *Let bounded potential $V \geq 0$ again suffice*

$$\lim_{R \rightarrow \infty} \|V\|_{L^\infty(\mathbb{R}^d \setminus B_R(0))} = 0,$$

then $\sigma_{disc}(H) = \emptyset$.

Proof. We know that $\forall \psi \in D(H) : (\psi, H\psi) = \int |\nabla \psi|^2 + \int V|\psi|^2 \geq 0$ and using the minimax principle (5.1.2) and the previous theorem we obtain $\min(\sigma(H)) \geq 0 \Rightarrow \sigma(H) = \sigma_{ess}(H) = [0, +\infty)$. \square

Since we use Minimax principle (Theorem 5.1.2) and Weyl's Theorem 5.1.1 in the first part of the proof, this statement applies only to self-adjoint operators. We will therefore focus on a more general approach that does not require self-adjointness.

5.3 Resolvents difference

Another, potentially more difficult to verify, condition for the stability of the essential spectrum results from the specific form of the difference of the resolvents. First, let us recall the definition of a resolvent function.

Definition 5.3.1 (Resolvent function). Resolvent function of operator A in \mathcal{H} is defined on resolvent set $\rho(A) \subset \mathbb{C}$ as $R_A(z) := (A - z)^{-1}$.

Resolvents difference can be used to secure stability of essential spectrum using following theorem [11].

Theorem 5.3.1 (Weyl's theorem). *Let A_1, A_2 be closed operators in \mathcal{H} such that $\exists \lambda \in \rho(A_1) \cap \rho(A_2)$, $(A_1 - \lambda)^{-1} - (A_2 - \lambda)^{-1} \in \mathcal{B}_\infty(\mathcal{H})$, then $\sigma_{ess}(A_1) = \sigma_{ess}(A_2)$.*

Unfortunately, this criterion can only be used for four of the five possible definitions of the essential spectrum from [11]. For the fifth and most commonly used definition, this does not apply in full generality. Here, however, we deal exclusively with sectorial operators [17], because we consider the potential relatively form-bounded with respect to free Hamiltonian. For sectorial operators, this also applies to the fifth definition of the essential spectrum due to the form of the resolvent set.

Let us adjust the resolvent difference of operators H_0 and H_V using resolvent identity to get a condition on the potential V . In order to do this we define the polar decomposition of the potential. We write the operator as a product of Hermitian positive semidefinite matrix and a unitary matrix:

$$V(x) = U(x)|V(x)|. \quad (5.6)$$

We also define

$$V_{\frac{1}{2}} := U(x)|V(x)|^{\frac{1}{2}} \quad (5.7)$$

and alter the decomposition as

$$V(x) = V_{\frac{1}{2}}(x)|V(x)|^{\frac{1}{2}}. \quad (5.8)$$

In short, we write it as $V = V_{\frac{1}{2}}|V|^{\frac{1}{2}}$. Now we can work with the resolvents difference using resolvent identity as well as this decomposition.

$$\begin{aligned} R_V(z) - R_0(z) &= -R_V(z)(H_V - H_0)R_0(z) \\ &= -R_V(z)VR_0(z)^{\frac{1}{2}}R_0(z)^{\frac{1}{2}} \\ &= -\underbrace{R_V(z)V_{\frac{1}{2}}}_{\text{bounded}}|V|^{\frac{1}{2}}\underbrace{R_0(z)^{\frac{1}{2}}R_0(z)^{\frac{1}{2}}}_{\text{bounded}}. \end{aligned}$$

Since the product of a bounded and compact operator is again a compact operator, it is enough to show that $|V|^{\frac{1}{2}}R_0(z)^{\frac{1}{2}}$ is compact. We also know that operator A is compact if and only if AA^* is compact, so we will continue to study $|V|^{\frac{1}{2}}R_0(z)|V|^{\frac{1}{2}}$. We can limit its Hilbert-Schmidt norm as

$$\| |V|^{\frac{1}{2}}R_0(z)|V|^{\frac{1}{2}} \|_{HS}^2 \leq \begin{cases} \frac{\|V\|_1^2}{4\sqrt{|z|}} & \text{for } d=1, \\ \int_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{|V(x)||V(y)|}{|x-y|^2} dx dy & \text{for } d=3. \end{cases} \quad (5.9)$$

$$\int_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{|V(x)||V(y)|}{|x-y|^2} dx dy \quad \text{for } d=3. \quad (5.10)$$

We can estimate the Hilbert-Schmidt norm because we know what resolvent kernel, the so-called Green's functions, look like in these dimensions:

$$g_\lambda(x, y) = \begin{cases} \frac{\exp(-\sqrt{-\lambda}|x-y|)}{2\sqrt{-\lambda}} & \text{for } d=1, \\ \frac{\exp(-\sqrt{-\lambda}|x-y|)}{4\pi|x-y|} & \text{for } d=3. \end{cases} \quad (5.11)$$

$$\frac{\exp(-\sqrt{-\lambda}|x-y|)}{4\pi|x-y|} \quad \text{for } d=3. \quad (5.12)$$

As Hilbert-Schmidt operators are compact, we just need to show that the expressions on the right hand side are finite. In case (5.9), it is sufficient that the potential is in the set $L^1(\mathbb{R})$. Then the Hilbert-Schmidt norm of $|V|^{\frac{1}{2}}R_0(z)|V|^{\frac{1}{2}}$ is finite and the operator is compact. Therefore, the resolvent difference is compact and the essential spectrum remains equal to the spectrum of the free Hamiltonian. It is worth recalling that this condition is in the first dimension a sufficient condition (see Proposition 3.4.1) for the correct introduction of the operator using the associated quadratic forms.

Similarly, for the case (5.10), the spectrum remains invariant if the right hand side is finite. This is achieved for the so-called Rollnik potentials [25].

Definition 5.3.2 (Rollnik potentials). We call operator V measurable in \mathbb{R}^3 a *Rollnik potential* ($V \in \mathcal{R}$) if

$$\|V\|_{\mathcal{R}} := \int_{\mathbb{R}^3 \times \mathbb{R}^3} \frac{|V(x)||V(y)|}{|x-y|^2} dx dy < \infty. \quad (5.13)$$

If we do not want to verify this condition directly, we can easily deduce a sufficient condition using the following theorem [20].

Theorem 5.3.2 (Hardy-Littlewood-Sobolev inequality). *For all λ , such that $0 < \lambda < d$, $\forall f \in L^p(\mathbb{R}^d)$ and $\forall g \in L^q(\mathbb{R}^d)$, where $p, q > 1 : \frac{\lambda}{d} + \frac{1}{p} + \frac{1}{q} = 2$, then $\exists C(d, \lambda, p)$ so that:*

$$\left| \int_{\mathbb{R}^d} \int_{\mathbb{R}^d} f(x) |x - y|^{-\lambda} g(y) dx dy \right| \leq C(d, \lambda, p) \|f\|_p \|g\|_q. \quad (5.14)$$

For our purposes $\lambda = 2, d = 3$ and $f = g = V$. Consequently, $V \in L^{\frac{3}{2}}(\mathbb{R}^3)$ is a sufficient condition for Rollnik potentials, i.e. $L^{\frac{3}{2}} \subset \mathcal{R}$. Moreover, this is in line with the result of the relative form-boundedness of potentials obtained from Sobolev inequality: $\|V\|_{L^{\frac{3}{2}}(\mathbb{R}^3)} < C$.

All of this reasoning works for scalar operator as well as for matrix operators. However to be absolutely precise, this should be done using associated quadratic forms instead of operators. That is because domain of operators H_0 and H_V do not equal, whereas domains of their associated forms do. So let's show the procedure for forms. First, we introduce the auxiliary vectors F and G :

$$G := (H_V - z) \psi, \quad (5.15)$$

$$F := (H_0 - z) \phi. \quad (5.16)$$

These definitions are equivalent to expressions

$$\psi = R_V(z)G, \quad (5.17)$$

$$\phi = R_0(z)F. \quad (5.18)$$

The resolvents difference will now be applied on the scalar product of vectors F, G as a form:

$$\begin{aligned} (F, [R_V(z) - R_0(z)]G) &= (F, R_V(z)G) - (R_0(z)F, G) \\ &= (F, \psi) - (\phi, G) \\ &= ((H_0 - z)\phi, \psi) - (\phi, (H_V - z)\psi) \\ &= (H_0 \phi, \psi) - (\phi, H_V \psi) \\ &= -(\phi, V\psi) \\ &= -\left(R_0(z)F, |V|^{\frac{1}{2}} V_{\frac{1}{2}} R_V(z)G \right) \\ &= -\left(F, [R_0(z)]^* |V|^{\frac{1}{2}} V_{\frac{1}{2}} R_V(z)G \right) \\ &= -\left(F, R_0(z) |V|^{\frac{1}{2}} V_{\frac{1}{2}} R_V(z)G \right). \end{aligned}$$

It follows from the equality that the expression is valid in the terms of forms and our procedure was therefore completely legitimate.

5.4 Rellich-Kondrachev theorem

Instead of estimating the Hilbert-Schmidt norm, we can use a more elegant procedure using the compact embedding theorem from [2].

Theorem 5.4.1 (Rellich-Kondrachov). *Let $\Omega \subseteq \mathbb{R}^d$ be an open, bounded Lipschitz domain, and let $1 \leq p < d$. Let*

$$p^* := \frac{dp}{d-p}.$$

Then

- $W^{1,p}(\Omega) \hookrightarrow L^{p^*}(\Omega)$ (continuous embedding),
- $W^{1,p}(\Omega) \subset\subset L^q(\Omega)$ for $1 \leq q < p^*$ (compact embedding).

Any potential vanishing in infinity can be approximated by the sequence of operators $\{V_m\}_{m=1}^\infty$ for which $\text{supp} V_m$ is compact. Therefore we have a bounded set $K_m := \text{supp} V_m$, we can use the previous theorem and we receive $H_0^1(K_m) \subset\subset L^2(K_m)$. Therefore, V_m is a compact operator for every $m \in \mathbb{N}$. We combine that with the fact that $R_0^{\frac{1}{2}} : L^2(\mathbb{R}^d) \rightarrow H^1(\mathbb{R}^d)$ is bounded. And since the product of a bounded and a compact operator is compact, we obtain a sequence of compact operators $\{V_m R_0^{\frac{1}{2}}\}_{m=1}^\infty$. Furthermore, we take advantage of the fact that the limit of a sequence of compact operators is again compact operator. If we combine this result with the previous section, we find that the difference of the resolvent is compact and therefore the essential spectrum does not change by adding such potential to the free Hamiltonian. This is possible substitute for the proof of Theorem 5.2.1, which works for matrix-valued potentials as well as non-Hermitian. Previous proofs allow us to state the following theorem.

Theorem 5.4.2. *Let us have function $V : \mathbb{C}^n \rightarrow \mathbb{C}^n$ acting as an operator of multiplication in $L^2(\mathbb{R}^d, \mathbb{C}^n)$. If this potential meets that*

- $V \in L^1(\mathbb{R})$ for $d = 1$,
- $V \in \mathcal{R}$ for $d = 3$,

then for operator $H_V = H_0 + V$ it holds that $\sigma_{\text{ess}}(H_V) = \sigma_{\text{ess}}(H_0) = \mathbb{R}_0^+$.

Chapter 6

Spectrum localization

Suppose we have a Schrödinger operator with a suitable potential. In the following text, that will denote potentials that meet the conditions for both the correct introduction of the operator and the stability of the essential spectrum. Of course, the specific conditions depend on the potential as well as on the physical dimension. We will first focus on the first dimension. Since in such a case we know the essential part of the spectrum, we want to examine the rest of it. So let's study the eigenvalue equation:

$$(H_0 + V)\psi = \lambda\psi \quad (6.1)$$

for $\psi \in D(H_V)$ and $V \in L^1(\mathbb{R}^d, \mathbb{C}^n)$.

6.1 Birman-Schwinger principle

First, we will examine the point spectrum in the dimension $d = 1$. In previous research [16], we have already modified estimate from [1] for matrix-valued potentials. However, the estimate was not optimal and did not apply eigenvalues in \mathbb{R}_0^+ , so we will improve it. We start by decomposing the potential as in the previous chapter, see (5.6):

$$V(x) = V_{\frac{1}{2}}(x)|V(x)|^{\frac{1}{2}}. \quad (6.2)$$

Next, we introduce the auxiliary operator K_λ and vector ϕ as

$$K_\lambda := |V|^{\frac{1}{2}}(-H_0 - \lambda)^{-1} V_{\frac{1}{2}}, \quad (6.3)$$

With them, we then rewrite the eigenvalues equation for $\lambda \notin [0, +\infty)$ and $\phi := -|V|^{\frac{1}{2}}\psi$.

$$K_\lambda\phi = -\phi. \quad (6.4)$$

This equivalency is known as the Birman-Schwinger principle. In order for the eigenvalue -1 to be in spectrum of K_λ there must exist respective vector ϕ such that $K_\lambda\phi = -\phi$ and therefore $\|K_\lambda\phi\| = \|\phi\|$, which yields

$$\|K_\lambda\| = \sup_{\psi} \frac{\|K_\lambda\psi\|}{\|\psi\|} \geq \frac{\|K_\lambda\phi\|}{\|\phi\|} = 1.$$

This provides us the lower estimation $\|K_\lambda\| \geq 1$. Next we derive upper estimation on the operator K_λ :

$$\begin{aligned} \|K_\lambda\|^2 &\leq \int_{\mathbb{R}^2} \|\mathcal{K}_\lambda(x, y)\|^2 dx dy \\ &\leq \int_{\mathbb{R}^2} |g_\lambda(x, y)|^2 \| |V(x)|^{\frac{1}{2}} V_{\frac{1}{2}}(y) \|^2 dx dy \\ &\leq \int_{\mathbb{R}^2} \frac{1}{4|\lambda|} \|V(x)\|_{\mathbb{C}^n} \|V(y)\|_{\mathbb{C}^n} dx dy. \end{aligned}$$

Integral kernel $\mathcal{K}_\lambda(x, y)$

$$\mathcal{K}_\lambda(x, y) = |V(x)|^{\frac{1}{2}} G_\lambda(x, y) V_{\frac{1}{2}}(y) \quad (6.5)$$

is defined using the matrix-valued Green function $G_\lambda = g_\lambda I$, where g_λ denotes its scalar form

$$g_\lambda(x, y) = \frac{e^{-\sqrt{-\lambda}|x-y|}}{2\sqrt{-\lambda}}. \quad (6.6)$$

Combining these two estimations creates a condition on eigenvalues of Schrödinger operator H_V outside of its essential spectrum.

Theorem 6.1.1 (Estimate for matrix potentials).

$$\lambda \in \sigma_p(H_V) \setminus [0, \infty) \quad \Rightarrow \quad |\lambda| \leq \frac{\| |V|_{\mathbb{C}^n} \|_{L^1(\mathbb{R})}}{4}. \quad (6.7)$$

Here norm $|V|_{\mathbb{C}^n}$ is standard matrix norm defined as

$$|V(x)|_{\mathbb{C}^n} := \|V(x)\|_{\mathbb{C}^n \rightarrow \mathbb{C}^n} = \sup_{u \in \mathbb{C}^n} \frac{\|V(x)u\|_{\mathbb{C}^n}}{\|u\|_{\mathbb{C}^n}}. \quad (6.8)$$

6.1.1 One-sided Birman-Schwinger principle

This estimate could be even stronger if we could use it to reduce the occurrence of eigenvalues from \mathbb{R}_0^+ as well. The classical Birman-Schwinger principle does not help us to do this, but its one-sided adjustment will. We define the same auxiliary operator K_λ with an integral kernel

$$\mathcal{K}_\lambda(x, y) = |V(x)|^{\frac{1}{2}} G_\lambda(x, y) V_{\frac{1}{2}}(y) \quad (6.9)$$

to help us solve the eigenvalue equation

$$H_V \psi = \lambda \psi \quad (6.10)$$

for $\lambda \in \mathbb{C}$ and $\psi \in D(H_V)$. To achieve this, we use one modification of the Birman-Schwinger principle for point spectrum.

Theorem 6.1.2 (Birman-Schwinger principle). *Let $H_V \psi = \lambda \psi$ for suitable potential V , $\psi \in D(H_V)$ and $\lambda \in \mathbb{C}$. Then there exists $\phi \in \mathcal{H}$ such that $\phi \neq 0$ if $\psi \neq 0$ and*

- (i) $K_\lambda \phi = -\phi$ if $\lambda \notin \sigma(H_0)$,
- (ii) $\lim_{\varepsilon \rightarrow 0} (\varphi, K_{\lambda+i\varepsilon} \phi) = -(\varphi, \phi)$ if $\lambda \in \sigma(H_0)$.

Extensive proof is to be found in [15]. To ensure its validity for matrix-valued potentials, let's go through the main idea of proof, namely $\forall \varphi \in L^2(\mathbb{R})$:

$$\lim_{\varepsilon \rightarrow 0} (\varphi, K_{\lambda+i\varepsilon} \phi) = -(\varphi, \phi).$$

It is appropriate to emphasize that λ is real and therefore $\lambda + i\varepsilon \notin \sigma(H_0)$ for all $\varepsilon \in \mathbb{R} \setminus \{0\}$. This means that the classic Birman-Schwinger principle applies to each operator $K_{\lambda+i\varepsilon}$. We will edit the expression within the limit

$$\begin{aligned} (\varphi, K_{\lambda+i\varepsilon} \phi) &= \int \int \overline{\varphi(x)} |V|^{\frac{1}{2}}(x) G_{\lambda+i\varepsilon}(x, y) V^{\frac{1}{2}}(y) \phi(y) dx dy \\ &= \int \mu_\varepsilon V(y) \psi(y) dy \end{aligned}$$

where

$$\mu_\varepsilon := \int \overline{\varphi(x)} |V|^{\frac{1}{2}}(x) G_{\lambda+i\varepsilon}(x, \cdot) dx = (H_0 - \lambda - i\varepsilon)^{-1} |V|^{\frac{1}{2}} \bar{\varphi} \in D(H_0)$$

and $\phi = |V|^{\frac{1}{2}} \psi$. Next, we use the form of the operator $H_V = H_0 + V$ and the eigenvalues equation $H_V \psi = \lambda \psi$:

$$\begin{aligned} (\varphi, K_{\lambda+i\varepsilon} \phi) &= -(\nabla \bar{\psi}, \nabla \mu_\varepsilon) + \lambda (\bar{\psi}, \mu_\varepsilon) \\ &= -(\nabla \bar{\psi}, \nabla \mu_\varepsilon) + (\lambda + i\varepsilon) (\bar{\psi}, \mu_\varepsilon) - i\varepsilon (\bar{\psi}, \mu_\varepsilon) \\ &= -(\bar{\psi}, |V|^{\frac{1}{2}} \bar{\varphi}) - i\varepsilon (\bar{\psi}, \mu_\varepsilon) \\ &= -(\varphi, |V|^{\frac{1}{2}} \psi) - i\varepsilon (\bar{\psi}, \mu_\varepsilon) \\ &= -(\varphi, \phi) - \underbrace{i\varepsilon (\bar{\psi}, \mu_\varepsilon)}_{\rightarrow 0} \rightarrow -(\varphi, \phi). \end{aligned}$$

Here the last relation holds because

$$\begin{aligned} \varepsilon (\bar{\psi}, \mu_\varepsilon) &= \varepsilon \left(|V|^{\frac{1}{2}} \bar{\phi}, (H_0 - \lambda - i\varepsilon)^{-1} |V|^{\frac{1}{2}} \bar{\varphi} \right) \\ &= \varepsilon \left(\bar{\phi}, |V|^{\frac{1}{2}} (H_0 - \lambda - i\varepsilon)^{-1} |V|^{\frac{1}{2}} \bar{\varphi} \right) \end{aligned}$$

and

$$\left| (\bar{\psi}, \mu_\varepsilon) \right| \leq \left\| |V|^{\frac{1}{2}} R_0(\lambda + i\varepsilon) |V|^{\frac{1}{2}} \right\|_{HS} \|\phi\| \|\varphi\|.$$

For L^1 potentials (see (5.9)):

$$\left\| |V|^{\frac{1}{2}} R_0(\lambda + i\varepsilon) |V|^{\frac{1}{2}} \right\|_{HS} \leq \frac{\|V\|_1^2}{4\sqrt{|\lambda + i\varepsilon|}}.$$

It follows that $\varepsilon(\bar{\psi}, \mu_\varepsilon)$ behaves at least as $O(\varepsilon^{1/2})$ and therefore

$$(\varphi, K_{\lambda+i\varepsilon}\phi) \xrightarrow{\varepsilon \rightarrow 0} -(\varphi, \phi).$$

The following theorem then replaces the lower bound from the previous section.

Theorem 6.1.3. *Let $H_V = H_0 + V$ with suitable potential and $\lambda \in \sigma_p(H_V)$.*

- (i) *If $\lambda \notin \sigma(H_0)$, then $\|K_\lambda\| \geq 1$.*
- (ii) *If $\lambda \in \sigma(H_0)$, then $\liminf_{\varepsilon \rightarrow 0} \|K_{\lambda+i\varepsilon}\| \geq 1$.*

Proof. (i) The claim (i) was shown in previous section using eigenvector ϕ :

$$\|K_\lambda\| = \sup_{\psi} \frac{\|K_\lambda\psi\|}{\|\psi\|} \geq \frac{\|K_\lambda\phi\|}{\|\phi\|} = 1.$$

- (ii) Let $\lambda \in \sigma(H_0)$ and $\lambda \in \sigma_p(H_V)$. We set $\phi_n := \xi_n\psi$ for $n \in \mathbb{N}$ and $\xi_n := \xi(x/n)$. Function $\xi \in \mathbb{C}_0^\infty$ satisfies $\xi(x) = 1$ for $|x| \leq 1$ and $\xi(x) = 0$ for $|x| \geq 2$. From Theorem 6.1.2 follows

$$\|\phi_n\| \|\phi\| \|K_{\lambda+i\varepsilon}\| \geq |(\phi_n, K_{\lambda+i\varepsilon}\phi)|.$$

Taking the limit $\varepsilon \rightarrow 0$ results in

$$\|\phi_n\| \|\phi\| \liminf_{\varepsilon \rightarrow 0} \|K_{\lambda+i\varepsilon}\| \geq |(\phi_n, \phi)|$$

and by taking the limit $n \rightarrow \infty$ we obtain the claim (ii). □

The upper estimate can be adjusted similarly and by combining them we obtain an estimate for all eigenvalues.

Theorem 6.1.4 (Improved estimate for matrix potentials). *Let $H_V = H_0 + V$ with $V \in L^1(\mathbb{R}, \mathbb{C}^n)$. Then*

$$\lambda \in \sigma_p(H_V) \quad \Rightarrow \quad |\lambda| \leq \frac{\| |V|^{\mathbb{C}^n} \|_{L^1(\mathbb{R})}}{4}. \quad (6.11)$$

6.1.2 Estimation optimality

Now it is time to verify that the estimate we have obtained for the operator's eigenvalues is optimal. To do this, we use the Dirac delta potential $\delta(x)$ and we have

$$H_\alpha := -\Delta + \alpha\delta(x). \quad (6.12)$$

Although this potential is obviously not integrable and therefore does not belong to the suitable potentials defined by us, it can be correctly introduced with the help of conditions on the domain of the operator $H_\alpha := -\frac{d^2}{dx^2}$. We limit its domain to $\varphi \in L^2(\mathbb{R}_-, \mathbb{C}^2) \oplus L^2(\mathbb{R}_+, \mathbb{C}^2)$ such that

$$\begin{aligned} \varphi_{1,2}(0-) &= \varphi_{1,2}(0+), \\ \varphi'_2(0-) &= \varphi'_2(0+), \\ \varphi'_1(0+) - \varphi'_1(0-) &= \alpha\varphi_1(0). \end{aligned}$$

Even more elegant solution is to use the associated forms and define the potential form as

$$v(\psi, \phi) := \alpha\overline{\psi(0)}\phi(0) \quad (6.13)$$

with $D(v) = W^{1,2}(\mathbb{R})$. The Schrödinger operator H_α is then m-sectorial operator associated with the form $h_\alpha = h_0 + v$. The eigenvalue problem for H_α can be solved explicitly

$$\lambda(\alpha) = -\frac{\alpha^2}{4}. \quad (6.14)$$

The norm of our matrix-valued delta potential is

$$\begin{aligned} \|V(x)\|_{\mathbb{C}^2} &= |\alpha|\delta(x) \\ \|\|V\|_{\mathbb{C}^2}\|_{L^1(\mathbb{R})}^2 &= \alpha^2. \end{aligned}$$

For this potential, we therefore found eigenvalue on the boundary of the circle defined by us in the complex plane. This shows that our estimate given by Theorem 6.1.4 is the best possible.

6.2 Third dimension

As we mentioned when defining conditions for potential, we typically deal with dimensions one and three. Our estimate given by Theorem 6.1.4 applies to the first dimension and now we will focus on what is happening in the third dimension. In such a case, the matrix Laplace operator is not a mere multiplication of its scalar form by a unit matrix, and the calculation is thus a bit more complicated. Fortunately, in the third dimension, the Green function of a free Hamiltonian has an explicit form, as we can find in [4]

$$G_\lambda(x, y) = \frac{\exp(-\sqrt{-\lambda}|x-y|)}{4\pi|x-y|}. \quad (6.15)$$

This function can be easily restricted from above as

$$|G_\lambda(x, y)| \leq G_0(x, y) = \frac{1}{4\pi|x-y|}, \quad (6.16)$$

but we will not obtain the same estimate as in previous section. Let's try different approach for third dimension.

In [14] it is shown, that for “small” potentials $V : \mathbb{R}^3 \rightarrow \mathbb{C}$ the spectrum of Schrödinger operator stays continuous and equal to positive real axis. We now modify this theorem for matrix-valued operators and show its validity.

Theorem 6.2.1. *Let $H = H_0 + V$, $V : \mathbb{R}^3 \rightarrow \mathbb{C}^n$ and there exists $a < 1$ so that $\forall u \in W^{1,2}(\mathbb{R}^3)$ holds that*

$$\int_{\mathbb{R}^3} |V||u|^2 dx \leq a \int_{\mathbb{R}^3} |\nabla u|^2 dx, \quad (6.17)$$

then $\sigma(H_V) = \sigma_c(H_V) = [0, +\infty)$.

The form of this condition is already known from Chapter 3 and tells us that the potential is relatively form-bounded with respect to the form of a free Hamiltonian with a relative bound less than one. From the previous chapter, we consider only potentials preserving the essential spectrum. The absence of the residual spectrum follows from \mathcal{T} -self-adjointness of the operator, see [5]. The Schrödinger operator is \mathcal{T} -self-adjoint [11] since it satisfies $H_V^* = H_{\overline{V}} = \mathcal{T}H_V\mathcal{T}$, where \mathcal{T} is the complex-conjugation operator defined as $\mathcal{T}\psi := \overline{\psi}$. To prove the claim, it is therefore sufficient for us to exclude the existence of all eigenvalues.

6.2.1 Point spectrum

To exclude the existence of eigenvalues, we use the extended Birman-Schwinger principle. We know from the previous procedures that the condition

$$\|K_\lambda\| \geq 1 \quad (6.18)$$

applies to the Birman-Schwinger operator. Therefore, if we show that

$$\|K_\lambda\| \leq a < 1 \quad (6.19)$$

also applies, we exclude the possibility of the existence of eigenvalues. Firstly, we write formulation equivalent to (6.17) in any dimension over 3 for $g = H_0^{-\frac{1}{2}}u$:

$$\| |V|^{\frac{1}{2}} H_0^{-\frac{1}{2}} g \|^2 \leq a \| \nabla H_0^{-\frac{1}{2}} g \|^2 = a \| g \|^2. \quad (6.20)$$

Since the range of $H_0^{-\frac{1}{2}}$ is dense in $L^2(\mathbb{R}^d)$, we can further see that

$$\| |V|^{\frac{1}{2}} H_0^{-\frac{1}{2}} \|^2 \leq a. \quad (6.21)$$

By using the adjoint, we also get

$$\|H_0^{-\frac{1}{2}} |V|^{\frac{1}{2}}\|^2 \leq a. \quad (6.22)$$

If we continue to limit ourselves to the third dimension and use the shape of the Green's function (6.15) and its limitation (6.16), we have

$$|(f, K_\lambda g)| \leq (|f|, K_0 |g|) \leq \|K_0\| \|f\| \|g\|, \quad (6.23)$$

where $f, g \in L^2(\mathbb{R}^3)$ and

$$K_0 = |V|^{\frac{1}{2}} H_0^{-1} V_{\frac{1}{2}}. \quad (6.24)$$

By combining the expressions (6.21) and (6.22) we get

$$\|K_0\| = \||V|^{\frac{1}{2}} H_0^{-1} V_{\frac{1}{2}}\| \leq \||V|^{\frac{1}{2}} H_0^{-1} |V|^{\frac{1}{2}}\| \leq \||V|^{\frac{1}{2}} H_0^{-\frac{1}{2}}\| \|H_0^{-\frac{1}{2}} |V|^{\frac{1}{2}}\|^2 \leq a. \quad (6.25)$$

Consequently,

$$\|K_\lambda\| \leq \|K_0\| \leq a. \quad (6.26)$$

This procedure is easily applicable to all eigenvalues $\lambda \notin [0, +\infty)$. To extend it to the real positive axis, the one-sided Birman-Schwinger principle is again used.

Conclusion

In the introduction to this work, we explained our motivation to study non-self-adjoint Schrödinger operators with matrix potentials. We have defined properties important for working with these operators, including properties for associated quadratic forms. It was with the help of these forms that we introduced the Schrödinger operator as the sum of the kinetic and the potential energy operators in the terms of forms.

To use such definition, it is customary that the potential is relatively form-bounded to free Hamiltonian with a relative bound less than one. We have derived sufficient conditions on the potential for this to apply. We also investigated these conditions for the magnetic energy operator.

Once we had a properly established operator, we focused on the spectrum. We examined the conditions of stability of the essential spectrum. From this we have derived groups of potentials for which the essential spectrum of the free Hamiltonian and the Schrödinger operator are the same. We have identified the two most important conditions on potentials, which correspond to the conditions from the previous section.

For operators with a known essential spectrum, we then focused on its eigenvalues. In the first dimension, we obtained an estimate using the modified Birman-Schwinger principle. In the third dimension, we then showed for which potentials the existence of eigenvalues can be ruled out.

These statements about the spectrum of matrix operators are another contribution to the theory of non-Hermitian quantum physics. They are especially suitable for the study of Pauli operators, where the situation is complicated by Pauli matrices. In the spirit of [6], the obtained results can be used to localize the eigenvalues of magnetic Dirac operators.

Bibliography

- [1] A. A. Abramov, A. Aslanyan, E. B. Davies: *Bounds on complex eigenvalues and resonances*. IOP-science, 2001.
- [2] R. A. Adams and J. J. F. Fournier, *Sobolev spaces*, Academic Press, 2003, 2nd edition.
- [3] F. Bagarello, J.P. Gazeau, F.H. Szafraniec, M. Znojil, (Eds.), *Non-selfadjoint operators in quantum physics: Mathematical aspects*, TN: John Wiley & Sons, Nashville, 2015.
- [4] J. Blank, P. Exner, M. Havlíček, *Lineární operátory v kvantové fyzice*, Karolinum, 1993.
- [5] D. Borisov and D. Krejčířík, *PT-symmetric waveguides*, Integ. Equ. Oper. Theory **62** (2008), 489–515.
- [6] L. Cossetti, L. Fanelli, D. Krejčířík. *Absence of eigenvalues of Dirac and Pauli Hamiltonians via the method of multipliers*, Comm. Math. Phys. 379 (2020), 633–691.
- [7] H. L. Cycon, R. G. Froese, W. Kirsch, B. Simon, *Schrödinger operators, with application to quantum mechanics and global geometry*, Springer-Verlag, Berlin, 2008.
- [8] E. B. Davies, *Linear Operators and their Spectra*, Cambridge University Press, Cambridge, 2007.
- [9] E.B. Davies, A. Hinz, *Kato class potentials for higher order elliptic operators*, J. London Math. Soc., 58 (2) (1998), 669–678.
- [10] L. Evans, *Partial Differential Equations* American Mathematical Society, Providence, R.I., 2010.
- [11] D. E. Edmunds and W. D. Evans, *Spectral theory and differential operators*, Oxford University Press, Oxford, 1987.
- [12] L. Fanelli, D. Krejčířík, *Location of eigenvalues of three-dimensional non-self-adjoint Dirac operators*, Lett. Math. Phys. 109 (2019) 1473–1485.
- [13] L. Fanelli, D. Krejčířík, L. Vega, *Absence of eigenvalues of two-dimensional magnetic Schrödinger operators*, J. Funct. Anal. 275 (2018), 2453–2472.
- [14] L. Fanelli, D. Krejčířík, L. Vega, *Spectral stability of Schrödinger operators with subordinated complex potentials*, J. Spectr. Theory 8, 575–604, 2018.
- [15] M. Hansmann, D. Krejčířík, *The abstract Birman-Schwinger principle and spectral stability*, arXiv:2010.15102, 2020.

- [16] M. Jaklinová, *Lokalizace vlastních hodnot Schrödingerových operátorů s maticovými potenciály*, CTU, Prague, 2018.
- [17] T. Kato: *Perturbation theory for linear operators*, Springer-Verlag, 1966.
- [18] D. Krejčířík, P. Siegl, *Elements of spectral theory without the spectral theorem in Non-selfadjoint Operators in Quantum Physics: Mathematical Aspects*, Wiley-Interscience, New York, 2015, p 241.
- [19] D. Krejčířík, P. Siegl, M. Tater, J. Viola, *Pseudospectra in non-Hermitian quantum mechanics*, J. Math. Phys. 56 (2015), 103513.
- [20] E. H. Lieb and M. Loss, *Analysis*, 2nd edn. AMS, Providence, 2001.
- [21] M. Reed and B. Simon, *Methods of modern mathematical physics, I. Functional analysis*, Academic Press, New York, 1972.
- [22] M. Reed and B. Simon, *Methods of modern mathematical physics, II. Fourier analysis. Selfadjointness*, Academic Press, New York, 1975.
- [23] M. Reed and B. Simon, *Methods of modern mathematical physics, IV. Analysis of operators*, Academic Press, New York, 1978.
- [24] M. Schechter, *Operator methods in quantum mechanics*, Elsevier, 1981.
- [25] B. Simon, *Quantum mechanics for Hamiltonians defined as quadratic forms*, Princeton Univ. Press, Princeton, 1971.
- [26] Q. Zheng and X. Quan, *Higher-order Kato class potentials for Schrödinger operators*, Bulletin of The London Mathematical Society **41** (2009), 293-301.