SPECTRAL THEORY FOR ONE-DIMENSIONAL THREE-BODY QUANTUM SYSTEMS

Master's Thesis in Mathematics
by Jonas Have

Supervisor: Horia Cornean

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Department of Mathematical Sciences
Aalborg University
Fredrik Bajers Vej 7G
9220 Aalborg Ø
http://www.math.aau.dk

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Jonas Have

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Abstract:

This thesis treats spectral theory for three-body quantum systems in one-dimension. Initially, a self-adjoint Schrödinger operator for a system with Dirac delta interactions is defined using a sesquilinear form. The exact domain of the Schrödinger operator is specified, and the essential spectrum is determined. To determine the essential spectrum a special case of the HVZ theorem is proven. Results regarding the resolvent of the Schrödinger operator is also proven. In the final chapter, another case of the three-body quantum system is considered. In this case, perturbation theory is used to determine the existence of a discrete eigenvalue and the behavior of this eigenvalue as a function of the coupling constant κ. It is shown that for small values of κ the behavior of the discrete eigenvalue is $\mathcal{O}(\kappa^4)$.

Preface

This report serves as my master's thesis and has been written during my final semester of the masters program in mathematics, at the department of Mathematical Sciences at Aalborg University. The subject of the report is spectral theory of three-body quantum systems in the mathematical physics framework.

In the report, I construct the Schrödinger Operator corresponding to a three-body quantum system in one-dimension with Dirac delta interactions. I give an explicit description of the domain of the operator and prove results regarding the resolvent operator. The thesis also contains proofs for results regarding the essential spectrum and perturbation theory.

I have tried to keep the thesis as self-contained as possible, but the reader is assumed to have basic knowledge of quantum mechanics, functional analysis and real and complex analysis.

All figures are produced in InkScape unless otherwise stated. Citations are denoted by square brackets with the authors name and the year of publication, e.g. [Reed and Simon, 1980]. The complete bibliography is found at the final page of the report. Vectors are denoted in bold, and the Euclidean norm of a vector $\mathbf{x}$ is denoted $|\mathbf{x}|$. An integral with no limits is, unless otherwise stated, the integral from $-\infty$ to $+\infty$.

Finally, I want to thank my supervisor Horia Cornean for allowing me to disturb him numerous times at his office, and his patient and excellent support during the project.

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Jonas Have
<jhave10@student.aau.dk>

Danish Summary

I dette speciale er der arbejdet med spektral teori for en-dimensionale kvante systemer bestående af to partikler med endelig masse, og en kerne med uendelig masse. Altså såkaldte tre-legeme systemer. Emnet er valgt ud fra en generel interesse i kvantemekanik og matematisk fysik, og på baggrund af tidligere arbejde med numeriske løsninger af lignende systemer.

I kvantemekanik repræsenteres observable af et system som selv-adjungerede operatorer. Med observable menes der egenskaber af et system som kan måles, det vil sige energi, position, impuls og så videre. Hamilton operatoren, også kaldet Schrödinger operatoren, repræsenterer energien af systemet. Spektret af Schrödinger operatoren består af de mulige energier af systemet. Energierne i det essetielle spektrum hører til spredningstilstandende, og de diskrete egenværdier hører til de såkaldte bundne tilstande.

Derfor er det første problem der arbejdes med, at konstruere en Schrödinger operator for systemet bestående af tre partikler der interagerer gennem Dirac delta distributioner. Af de tre partikler i systemet har to partikler endelig masse, og den sidste uendelig masse. Schrödinger operatoren, herefter noteret H, konstrueres ud fra en sesquilinear form. Til dette anvendes en udgave af Lax-Milgrams sætning. En præcis beskrivelse af domænet af H gives til slut i Kapitel 2. I Kapitel 3 ønskes det essentielle spektrum af H bestemt. Til dette anvendes Hunziker - van Winter - Zhislin sætningen, eller HVZ sætningen. En del af arbejdet i Kapitel 3 går med at bevise at sætningen holder for systemet repræsenteret ved H. Kapitel 4 omhandler resolventen af $H - z$ og den såkaldte frie resolvent. Der bevises en sætning der kan anvendes til at bestemme de diskrete egenværdier, men selve bestemmelsen af egenværdierne er dog udeladt. Denne del af specialet er udarbejdet med udgangspunkt i artiklen [Cornean et al., 2006].

Det sidste problem der arbejdes med i specialet omhandler en anden variation af tre-legeme systemet. I dette system har de to partikler med endelig masse modsat ladning. Derudover anvendes ikke længere Dirac delta interaktioner, men i stedet en glat interaktions funktion. Der anvendes perturbations teori på dette problem, specifikt anvendes Feshbachs formel. Til sidst vises eksistensen af en diskret

egenværdi, og dennes opførsel som funktion af koblings konstanten. Systemet der arbejdes med i denne del af rapporten har interesse, da det kan anvendes som en model for excitoner i en-dimensionale halvledere.

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Chapter 1

Introduction

In this chapter, we want to give a short introduction to the problems and theory which we consider. The thesis is written in the mathematical physics framework. Mathematical physics is the study of physical theories in a mathematically rigorous framework.

The mathematical description of quantum mechanics is contained in the axioms which were formulated by Dirac 1930 and refined by von Neumann in 1932. The axioms state among other things that the state of a quantum system is represented by a unit vector $\psi \in \mathcal{H}$, where $\mathcal{H}$ is a Hilbert space. The axioms also state that the observables of a quantum system are the set of self-adjoint operators on $\mathcal{H}$, and finally that the expectation value of an observable A in state ψ is given by the inner product $\langle \psi, A\psi \rangle$. See e.g. [Hall, 2013].

Suppose we want to describe the energy of a non-relativistic particle moving in a potential described by V. Inspired by the Hamiltonian from classical mechanics the energy operator has a kinetic energy term and a potential energy term. Using atomic units the quantum mechanical energy operator can be written as

$$-\frac{1}{2}\Delta + V, \tag{1.1}$$

on the Hilbert space L^2, and where Δ is the Laplacian operator. The energy operator is usually called the Schrödinger operator in mathematical physics and the Hamiltonian operator in physics. We will use the mathematical expression and call it the Schödinger operator.

The systems we consider consist of three spinless nonrelativistic particles in one-dimension with no external potential. All the systems we study are systems of nonrelativistic spinless particles, and we will, therefore, refrain from mentioning that they are nonrelativistic and spinless again. Since the system has no external potential, the potential is simply due to the interparticle interaction. If $v_{ij}(x_i - x_j)$ denotes the interaction between particles x_i and x_j, then the energy operator for this type of system must be of the type

$$H = -\frac{1}{2}\sum_{i=1}^{3}\frac{\partial^2}{\partial x_i^2} + \sum_{1\le i<j\le 3} v_{ij}(x_i - x_j) \tag{1.2}$$

where x_1, x_2, x_3 denotes the position of the particles. For a given systems, the first problem that might be encountered is showing that a Schrödinger operator actually does exist, for that given system, and that it is self-adjoint. When the existence of the Schrödinger operator H has been shown determining the possible energies of the system is equivalent to the determination of the spectrum of H. The spectrum can be decomposed into a discrete spectrum and the essential spectrum, which we will define later. The discrete spectrum corresponds to the bound states of the system, and the essential spectrum corresponds to the scattering states.

At first, the thought of one-dimensional quantum systems might seem like a mathematical abstraction with little to no physical meaning and no actual applications. But as argued in [Pedersen, 2015] the one-dimensional systems appear for instance in the study of quantum wires and carbon nanotubes. The case of excitons in carbon nanotubes was treated in the article [Cornean et al., 2004].

1.1 Outline

We give here a short outline of the thesis.

In Chapter 2 we show the existence of a Schrödinger operator for a system with Dirac delta interactions. Using the Lax-Milgram theorem we can associate a Schrödinger operator H to a sesquilinear form, and show that the operator is self-adjoint. The chapter is concluded with a description of the domain of H.

The next chapter addresses the determination of the essential spectrum of H. The essential spectrum is determined using the HVZ theorem. The bulk of Chapter 3 is proving the HVZ theorem for the actual system we consider. Chapter 4 is about the resolvent of H and the free resolvent. The main result from Chapter 4 serves as a starting point for proving the existence of a discrete spectrum of H. We leave out showing the existence of a discrete spectrum for H. This part of the thesis is inspired by the work presented in [Cornean et al., 2006].

Chapter 5 deals perturbation theory for a system with interaction $v \in C_0^\infty$, instead of the Dirac delta interaction. The Feshbach formula and the Birman-Schwinger principle is used to show the existence of a discrete eigenvalue. Furthermore, the leading behavior of the eigenvalue is determined. In addition, an appendix with miscellaneous results is included at the end of the report. The results are predominantly from functional analysis and are included simply to keep the thesis as a self-contained as possible.

Chapter 2

Construction of the Schrödinger Operator

In this chapter, we will construct the Schrödinger operator of a system consisting of a nucleus with infinite mass and two finite particles with finite mass. The particles move in one dimension, and the particle interaction is modeled by the Dirac delta distribution. As mentioned in Chapter 1 the Schrödinger operator of a three-body system is given by (1.2). If one of the particles have infinite mass there is no kinetic energy associated with that particle. Consequently, the Schrödinger operator of the system have the form

$$H = -\frac{1}{2}\frac{\partial^2}{\partial x^2} - \frac{1}{2}\frac{\partial^2}{\partial y^2} + \lambda_1\delta(x) + \lambda_2\delta(y) + \lambda_3\delta(x-y), \tag{2.1}$$

where x, y are the position of the particles with finite mass and $\lambda_1, \lambda_2, \lambda_3 \in \mathbb{R}$. The coefficients λ_1, λ_2 and λ_3 model the strength of the interparticle interactions, and whether the interaction is repulsive or attractive.

We define the Schrödinger operator in (2.1) as the self-adjoint operator associated with the sesquilinear form $Q(\cdot,\cdot)$ defined on $H^1(\mathbb{R}^2)$, the first Sobolev Space defined in Definition A.3.2. The sesquilinear form Q is given by

$$\begin{aligned} Q(f,g) = \frac{1}{2}\iint \overline{\nabla f(x,y)} \cdot \nabla g(x,y)\,\mathrm{d}x\,\mathrm{d}y + \lambda_1 \int \overline{f(x,0)}g(x,0)\,\mathrm{d}x \\ + \lambda_2 \int \overline{f(0,y)}g(0,y)\,\mathrm{d}y + \lambda_3 \int \overline{f(x,x)}g(x,x)\,\mathrm{d}x, \end{aligned} \tag{2.2}$$

where $\lambda_1, \lambda_2, \lambda_3 \in \mathbb{R}$. Note that we use the convention from physics where the form is anti-linear in the first argument, and linear in the second argument. We will keep this convention through the whole report.

There are a few formalities which need to be in place before we construct the operator. First of all, we need to show that functions of the type $f(x,0), f(0,y)$

and $f(x,x)$ can be properly defined for functions in $H^1(\mathbb{R}^2)$. Next, we need to show which properties a sesquilinear form should satisfy for us to be able to associate a unique self-adjoint operator with it. Finally, we need to show that Q indeed does have these properties. At the end of the chapter, we will have shown that the operator H in (2.1) is the self-adjoint operator associated with the sesquilinear form Q. Additionally, in the final section of the chapter, we give a precise description of the domain of H.

2.1 Restrictions to hyperplanes

The first thing we need to consider before constructing the Schrödinger operator is the definition of expressions such as $f(x,0), f(0,y)$ and $f(x,x)$. We show that such functions can be properly defined for functions in $H^1(\mathbb{R}^2)$. This discussion can obviously be generalized to functions $f : \mathbb{R}^d \to \mathbb{R}$ which are restricted to hyperplanes of $\mathbb{R}^d$. The section is based on results from section IX.9 in [Reed and Simon, 1975].

Note first that for $f \in L^2(\mathbb{R}^d)$, the restriction of to a hyperplane of $\mathbb{R}^d$ does not have to be defined. This follows since the Lebesgue measure of a hyperplane in $\mathbb{R}^d$ is zero and L^2-functions are not necessarily defined on sets with measure zero. Instead, we show that functions in the Sobolev space $H^1(\mathbb{R}^d)$ can be restricted to a hyperplane M of $\mathbb{R}^d$.

We only need the case $d = 2$. In $d = 2$ the hyperplane is a line, and without loss of generality we can assume that the hyperplane is $M = \{(x,0) : \forall x \in \mathbb{R}\}$. If $f \in H^1(\mathbb{R}^2)$, then the direct restriction of f on M might not be well defined since $H^1(\mathbb{R}^2) \not\subset C^0(\mathbb{R}^2)$. Sobolev's lemma, Theorem A.3.4, shows that $H^s(\mathbb{R}^2) \subset C^0(\mathbb{R}^2)$ for $s > 1$. But it does not tell us whether $H^1(\mathbb{R}^2) \subset C^0(\mathbb{R}^2)$. Actually it is possible to construct functions $f \in H^1(\mathbb{R}^2)$, which are not in $C^0(\mathbb{R}^2)$. Luckily we can avoid this problem by using Theorem A.3.5, which states that $C^\infty(\mathbb{R}^2) \cap H^1(\mathbb{R}^2)$ is dense in $H^1(\mathbb{R}^2)$.

For $f \in H^1(\mathbb{R}^2)$ use Theorem A.3.5 to choose a sequence $\{f_n\} \in C^\infty(\mathbb{R}^2) \cap H^1(\mathbb{R}^2)$ such that

$$\|f_n - f\|_{H^1} \to 0, \quad \text{for } n \to \infty. \tag{2.3}$$

Since $f_n \in C^\infty$ the restriction $f(x,0)$ is well defined. Then we define the sequence $\{g_n\}$, with g_n given by

$$g_n(x) := f(x,0) = \frac{1}{2\pi} \int e^{ik_1 x} \hat{f}_n(\boldsymbol{k})\, \mathrm{d}\boldsymbol{k}, \tag{2.4}$$

where $\boldsymbol{k} = (k_1, k_2)$ and $\mathrm{d}\boldsymbol{k} = \mathrm{d}k_1\, \mathrm{d}k_2$. We show that $g_n \in L^2(\mathbb{R})$ for all n, and that $\{g_n\}$ is a Cauchy sequence. If $\{g_n\}$ is a Cauchy sequence it converges to a unique limit $g \in L^2(\mathbb{R})$, since $L^2(\mathbb{R})$ is a Hilbert space. First consider

$$
\begin{aligned}
|g_n(x)| &\le \frac{1}{2\pi} \int \left| \int e^{ik_1x} \hat{f}_n(\boldsymbol{k}) \, \mathrm{d}k_1 \right| \mathrm{d}k_2 && (2.5)\\
&= \frac{1}{2\pi} \int \frac{(1+k_2^2)^{1/2}}{(1+k_2^2)^{1/2}} \left| \int e^{ik_1x} \hat{f}_n(\boldsymbol{k}) \, \mathrm{d}k_1 \right| \mathrm{d}k_2 && (2.6)\\
&\le \frac{1}{2\pi} \left(\int \frac{\mathrm{d}k_2}{1+k_2^2} \right)^{1/2} \left(\int (1+k_2^2) \left| \int e^{ik_1x} \hat{f}_n(\boldsymbol{k}) \, \mathrm{d}k_1 \right|^2 \mathrm{d}k_2 \right)^{1/2}. && (2.7)
\end{aligned}
$$

The final inequality follows from the Cauchy-Schwarz inequality. Next, we consider

$$
\begin{aligned}
\int |g_n(x)|^2 \, \mathrm{d}x &= \frac{C}{\sqrt{2\pi}} \iint (1+k_2^2) \left| \int e^{ik_1x} \hat{f}_n(\boldsymbol{k}) \, \mathrm{d}k_1 \right|^2 \mathrm{d}k_2 \, \mathrm{d}x && (2.8)\\
&= C \iint (1+k_2^2) |\hat{f}_n(\boldsymbol{k})|^2 \, \mathrm{d}\boldsymbol{k} && (2.9)\\
&\le C \|f_n\|_{H^1} < \infty, && (2.10)
\end{aligned}
$$

for some constant $C > 0$. The second equality follows from the Plancherel theorem, Theorem 9.13 in [Rudin, 1987]. We see that g_n is indeed in $L^2(\mathbb{R})$. Repeating the calculations for $\|g_n - g_m\|_{L^2}$ and applying

$$
\|(1+|\boldsymbol{k}|^2)^{\frac{1}{2}} (\hat{f}(\boldsymbol{k}) - \hat{f}_n(\boldsymbol{k}))\|_{L^2} \to 0, \quad \text{for } n \to \infty, \tag{2.11}
$$

which follows from the definition of Sobolev spaces, we can show that $\{g_n\}$ is a Cauchy sequence in $L^2(\mathbb{R})$. Thus it converges to a unique $g \in L^2(\mathbb{R})$. We define $f(x,0) := g(x)$.

The following theorem follows from the discussion above.

Theorem 2.1.1 *Let $f \in \mathscr{S}(\mathbb{R}^2)$, where $\mathscr{S}(\mathbb{R}^2)$ is the Schwartz space in Definition A.3.1. Aditionally, let $T_M f$ be the restriction of f to a hyperplane M in $\mathbb{R}^2$. Then T_M extends uniquely to a bounded map $\tau : H^1(\mathbb{R}^2) \to L^2(\mathbb{R})$. We call τ the trace operator.*

Using Theorem 2.1.1 it is now possible to restrict functions in $H^1(\mathbb{R}^2)$ to a line, and the restriction is in $L^2(\mathbb{R})$. Thus, the sesquilinear form Q given by (2.2) is defined on $H^1(\mathbb{R}^2)$.

2.2 Lax-Milgram Theorem and Self-Adjoint Operators

In this section, we introduce the Lax-Milgram theorem and give a method for associating to sesquilinear forms self-adjoint operators. The proofs in this section are inspired by proofs in the notes [Helffer, 2010].

Let Q be a sesquilinear form defined on $\mathcal{H} \times \mathcal{H}$, where $\mathcal{H}$ is a Hilbert space. We begin by defining a specific property of a sesquilinear form.

Definition 2.2.1
Let $Q : \mathcal{H} \times \mathcal{H} \to \mathbb{C}$ be a sesquilinear form, and $\mathcal{H}$ a Hilbert space. Then Q is said to be coercive on $\mathcal{H}$ if there exists $\delta > 0$ such that

$$|Q(f,f)| \geq \delta \|f\|^2, \quad \forall f \in \mathcal{H}. \tag{2.12}$$

Recall, that a sesquilinear form Q on $\mathcal{H} \times \mathcal{H}$ is continuous if and only if there exists a constant $C > 0$ such that

$$|Q(f,g)| \leq C \|f\| \|g\|, \quad \forall f, g \in \mathcal{H}. \tag{2.13}$$

If Q is a continuous sesquilinear form, then Riesz representation theorem, Theorem A.1.5, gives the existence of a bounded operator T on $\mathcal{H}$ such that

$$Q(f,g) = \langle f, Tg \rangle, \quad \forall f, g \in \mathcal{H}. \tag{2.14}$$

With these properties in place, we are ready to state the Lax-Milgram theorem.

Theorem 2.2.2 (Lax-Milgram Theorem) *Let $\mathcal{H}$ be a Hilbert space and Q a continuous and coercive sesquilinear form on $\mathcal{H} \times \mathcal{H}$. Then the map T, given by* (2.14)*, is an isomorphism from $\mathcal{H}$ onto $\mathcal{H}$.*

Proof. Since Q is coercive on $\mathcal{H}$, we have that for some $\delta > 0$

$$\delta \|f\|^2 \leq |Q(f,f)| = |\langle f, Tf \rangle| \leq \|Tf\| \|f\|, \quad \forall f \in \mathcal{H}. \tag{2.15}$$

This shows that $\delta \|f\| \leq \|Tf\|$. Thus, T the inverse of T exists.

We want to prove that the range of T, denoted by $R(T)$, is equal to $\mathcal{H}$. Let $\{Tf_k\} \subset R(T)$ be a convergent sequence with a limit $g \in \mathcal{H}$. Then by the coercivity of Q there exists $\delta > 0$ such that

$$\delta \|f_n - f_m\| \leq \|Tf_n - Tf_m\|. \tag{2.16}$$

Then $\{f_k\}$ is a Cauchy sequence, and hence convergent to a limit $f \in \mathcal{H}$. The continuity of T gives that $Tf = g \in R(T)$. We have showed that $R(T)$ is a closed subset of $\mathcal{H}$. Assume that $R(T) \neq \mathcal{H}$, then Theorem A.1.2 guarantees the existence of a nonzero $g \in \mathcal{H}$ such that

$$\langle g, Tf \rangle = 0, \quad \forall f \in \mathcal{H}. \tag{2.17}$$

But by coercivity of Q there exists $\delta > 0$ such that $\delta \|g\|^2 \leq Q(g,g) = \langle g, Tg \rangle = 0$, since (2.17) holds for all $f \in \mathcal{H}$, including g. But this implies that $g = 0$, which is contradiction. So we have that $R(T) = \mathcal{H}$.

Finally we show that T^{-1} is bounded. For all $g \in \mathcal{H}$, there exists $f \in \mathcal{H}$ such that $f = T^{-1}g$. Then the coercivity of Q gives that there exists $\delta > 0$ such that

$$\delta \|f\| = \delta \|T^{-1}g\| \leq \|Tf\| = \|g\|. \tag{2.18}$$

Which shows the boundedness of T^{-1}. □

We now consider the Hilbert spaces $\mathcal{V}$ and $\mathcal{H}$, where $\mathcal{V} \subset \mathcal{H}$. We assume that there exists a constant $C > 0$ such that

$$\|f\|_{\mathcal{H}} \leq C\|f\|_{\mathcal{V}}, \quad \forall f \in \mathcal{V}. \tag{2.19}$$

Furthermore we assume that $\mathcal{V}$ is dense in $\mathcal{H}$. We can then associate to a sesquilinear form Q, which is coercive on $\mathcal{V}$, an unbounded operator S on $\mathcal{H}$. First we define the domain of S as

$$D(S) := \{g \in \mathcal{V} : \exists C > 0 \text{ s.t. } |Q(f,g)| \leq C\|f\|_{\mathcal{H}}\|g\|_{\mathcal{H}}, \forall f \in \mathcal{V}\}. \tag{2.20}$$

Then using Riesz representation, and the assumption that $\mathcal{V}$ is dense in $\mathcal{H}$, we can define $Sg \in \mathcal{H}$ by

$$Q(f,g) = \langle f, Sg\rangle_{\mathcal{H}}, \quad \forall f \in \mathcal{V}. \tag{2.21}$$

This leads us to the next result.

Theorem 2.2.3 *Let $\mathcal{V}$ and $\mathcal{H}$ be Hilbert spaces satisfying the assumptions mentioned previously, and let S be the map defined by* (2.21). *Then S is bijective from $D(S)$ onto $\mathcal{H}$ and S^{-1} is a bounded linear map on $\mathcal{H}$. Furthermore, $D(S)$ is dense in $\mathcal{H}$.*

Proof. The proof is quite similar to the proof of Lax-Milgram's theorem, but with a few subtle differences. First we prove that S is an injective map from $D(S)$ to $\mathcal{H}$. Let $\delta > 0$ be given by the coercivity of Q on $\mathcal{V}$ and consider

$$\delta\|f\|^2_{\mathcal{H}} \leq C\delta\|f\|^2_{\mathcal{V}} \leq C|Q(f,f)| = C|\langle f, Sf\rangle_{\mathcal{H}}| \leq C\|Sf\|_{\mathcal{H}}\|f\|_{\mathcal{H}}, \tag{2.22}$$

for all $f \in D(S)$ and $C > 0$. Then $\delta\|f\|_{\mathcal{H}} \leq C\|Sf\|_{\mathcal{H}}$ for all $f \in D(S)$, this proves that S is injective. Next we show that S is a surjective map. If $h \in \mathcal{H}$ then $\langle \cdot, h\rangle_{\mathcal{H}}$ defines a linear functional on $\mathcal{V}$. Then Riesz representation guarantees the existence of a unique $g \in \mathcal{V}$ such that

$$\langle f, h\rangle_{\mathcal{H}} = \langle f, g\rangle_{\mathcal{V}}, \quad \forall f \in \mathcal{V}. \tag{2.23}$$

Lax-Milgram's theorem gives the existence of a map T such that $w = T^{-1}g \in \mathcal{V}$, and which satisfies

$$Q(f,w) = \langle f, g\rangle_{\mathcal{V}}, \quad \forall f \in \mathcal{V}. \tag{2.24}$$

But then w must be in $D(S)$ since

$$Q(f,w) = \langle f, h\rangle_{\mathcal{H}}, \quad \forall f \in \mathcal{V}, \tag{2.25}$$

and $Sw = h$. It follows that $h \in R(S)$ and since h was arbitrary S is surjective on $\mathcal{H}$. The continuity of S^{-1} comes from the inequality $\delta\|f\|_{\mathcal{H}} \leq C\|Sf\|_{\mathcal{H}}$.

Finally, we need to show that $D(S)$ is dense in $\mathcal{H}$. If $D(S)$ is dense in $\mathcal{H}$, then $\overline{D(S)} = \mathcal{H}$ and $D(S)^{\perp} = \{0\}$. We take an element in $f \in \mathcal{H}$ such that

$$\langle g, f\rangle_{\mathcal{H}} = 0, \quad \forall g \in D(S). \tag{2.26}$$

But since S is surjective on $\mathcal{H}$ we can find $h \in D(S)$ such that $f = Sh$. Then by (2.26), we must have that $\langle Sh, h\rangle_{\mathcal{H}} = 0$. But then the coercitivity of Q implies that $f = 0$. This concludes the proof. □

We now introduce a result which shows when the operator associated to a sesquilinear form is self-adjoint.

Theorem 2.2.4 *Let Q be the sesquilinear form used to define the operator S in* (2.21)*. If Q is symmetric, then*

1. *S is closed*
2. *S is self-adjoint*
3. *$D(S)$ is dense in $\mathcal{V}$.*

Proof. We begin by proving statement 2. Note that if Q is symmetric, then S is a symmetric operator. But S symmetric implies that

$$D(S) \subseteq D(S^*). \tag{2.27}$$

Take $f \in D(S^*)$. By Theorem 2.2.3 we have that S is surjective, then there must exist a $f_0 \in D(S)$ such that

$$Sf_0 = S^* f. \tag{2.28}$$

The symmetry of S and the definition of an adjoint operator gives

$$\langle f_0, Sg\rangle = \langle Sf_0, g\rangle = \langle S^* f, g\rangle = \langle f, Sg\rangle, \quad \forall g \in D(S). \tag{2.29}$$

But then $\langle Sg, f_0 - f\rangle = 0$ for all $g \in D(S)$. Since S is surjective we have that $f_0 = f$. This implies that $D(S) = D(S^*)$ and $Sf = S^* f$ for all $f \in D(S)$. Then S is self-adjoint. Statement 1. follows from Theorem VIII.1 in [Reed and Simon, 1980] which tells us that S^* is closed. Thus, S is closed since it is self-adjoint.

Finally, we prove statement 3. Let $f \in \mathcal{V}$ such that

$$\langle f, g\rangle_{\mathcal{V}} = 0, \quad \forall g \in D(S). \tag{2.30}$$

By Lax-Milgram's theorem we have a linear map A which is an isomorphism of $\mathcal{V}$ onto $\mathcal{V}$. Then we can write $f = Ah$ for some $h \in \mathcal{V}$. Then we have

$$0 = \langle Ah, g\rangle_{\mathcal{V}} = \overline{\langle g, Ah\rangle_{V}} = \overline{Q(g,h)} = Q(h,g) = \langle h, Sg\rangle_{\mathcal{H}}, \quad \forall g \in D(S). \tag{2.31}$$

But since S is a surjective map we must have $h = 0$, and consequently $f = 0$. Then $D(S)$ is dense in $\mathcal{V}$. □

In this section we have shown how to associate operators to sesquilinear forms, and what the sesquilinear form needs to satisfy for the operator to be self-adjoint.

2.3 Construction of the operator

We are now ready to show that a self-adjoint operator can be associated to the sesquilinear form given by (2.2).

We begin by defining another sesquilinear form $\tilde{Q}$ on $H^1(\mathbb{R}^2) \times H^1(\mathbb{R}^2)$. We then show that we can associate a self-adjoint operator to the form $\tilde{Q}$, and afterward use this to associate a self-adjoint operator to the sesquilinear form in (2.2). Define $\tilde{Q}$ by

$$\begin{aligned}\tilde{Q}(f,g) = \frac{1}{2}\iint \overline{\boldsymbol{\nabla} f(x,y)} \cdot \boldsymbol{\nabla} g(x,y)\,\mathrm{d}x\,\mathrm{d}y + \lambda_1 \int \overline{f(x,0)} g(x,0)\,\mathrm{d}x \\ + \lambda_2 \int \overline{f(0,y)} g(0,y)\,\mathrm{d}y + \lambda_3 \int \overline{f(x,x)} g(x,x)\,\mathrm{d}x + \lambda \langle f, g\rangle_{L^2}, \quad (2.32)\end{aligned}$$

where $\lambda > 0$ and $\lambda_1, \lambda_2, \lambda_3 \in \mathbb{R}$.

We want to apply Theorem 2.2.3 and the associated result from Theorem 2.2.4 to construct a self-adjoint operator. To apply Theorem 2.2.3, we note that $H^1(\mathbb{R}^2)$ is dense in $L^2(\mathbb{R}^2)$ and that

$$\|f\|_{L^2} \le \|f\|_{H^1}, \quad \forall f \in H^1(\mathbb{R}^2). \quad (2.33)$$

So we just need to show that $\tilde{Q}$ is coercive and continuous on $H^1(\mathbb{R}^2)$ to apply Theorem 2.2.3. To show that, we need the following lemma.

Lemma 2.3.1 *Let $f \in H^1(\mathbb{R}^2)$. Then the following identity holds*

$$\int |f(x,0)|^2\, dx \le \varepsilon C \|f\|_{H^1}^2 + \frac{C}{\varepsilon}\|f\|_{L^2}^2, \quad \forall \varepsilon > 0, \quad (2.34)$$

where $C > 0$.

Proof. The proof follows from direct calculations similar to those before Theorem 2.1.1 so we skip some of the details. Take $M > 0$ and write $(M + k_2^2)$ in the final inequality in (2.5), then we have

$$|f(x,0)| \le \frac{1}{2\pi}\left(\int \frac{\mathrm{d}k_2}{M + k_2^2}\right)^{1/2} \left(\int (M + k_2^2)\left|\int e^{ik_1 x}\hat{f}(\boldsymbol{k})\,\mathrm{d}k_1\right|^2 \mathrm{d}k_2\right)^{1/2}.$$

Substituting $k_2 = \sqrt{M}x$, in the first integral we find

$$|f(x,0)| \le \frac{1}{2\pi}\left(\frac{C}{\sqrt{M}}\right)^{1/2} \left(\int (M + k_2^2)\left|\int e^{ik_1 x}\hat{f}(\boldsymbol{k})\,\mathrm{d}k_1\right|^2 \mathrm{d}k_2\right)^{1/2}. \quad (2.35)$$

Using Plancherel's theorem we find that

$$\begin{aligned}\int |f(x,0)|^2\,\mathrm{d}x &\le \frac{C}{\sqrt{M}}\int (M+|\boldsymbol{k}|^2)|\hat{f}(\boldsymbol{k})|^2\,\mathrm{d}\boldsymbol{k}. \\ &= \frac{C}{\sqrt{M}}\left((M-1)\int |\hat{f}(\boldsymbol{k})|^2\,\mathrm{d}\boldsymbol{k} + \int (1+|\boldsymbol{k}|^2)|\hat{f}(\boldsymbol{k})|^2\,\mathrm{d}\boldsymbol{k}\right) \\ &\le C\sqrt{M}\|f\|_{L^2}^2 + \frac{C}{\sqrt{M}}\|f\|_{H^1}^2.\end{aligned} \tag{2.36}$$

Since this holds for arbitrary $M > 0$, we have that (2.34) holds for all $\varepsilon > 0$. □

Note that equivalent results holds for $f(x,0)$ and $f(x,x)$. From the previous result it is also obvious that the following inequlity holds for some constant $C > 0$.

$$\left(\int |f(x,0)|^2\,\mathrm{d}x\right)^{1/2} \le \varepsilon C\|f\|_{H^1} + \frac{C}{\varepsilon}\|f\|_{L^2}, \quad \forall\varepsilon > 0. \tag{2.37}$$

We are now ready to show that $\tilde{Q}$ is continuous and coercive on $H^1(\mathbb{R}^2)$. We begin by showing continuity, that is $|\tilde{Q}(f,g)| \le C\|f\|_{H^1}\|g\|_{H^1}$ for some constant $C > 0$ and for all $f, g \in H^1(\mathbb{R}^2)$. Using the Cauchy-Schwarz inequality and Lemma 2.3.1 we see that

$$\begin{aligned}|\tilde{Q}(f,g)| &\le \|f\|_{H^1}\|g\|_{H^1} + 3C^2(\varepsilon\|f\|_{H^1} + \varepsilon^{-1}\|f\|_{L^2})(\varepsilon\|g\|_{H^1} + \varepsilon^{-1}\|g\|_{L^2}) \\ &\quad + \lambda\|f\|_{L^2}\|g\|_{L^2} \\ &\le (1 + 3C^2(\varepsilon^2 + \varepsilon^{-2} + 2) + \lambda)\|f\|_{H^1}\|g\|_{H^1} = \tilde{C}\|f\|_{H^1}\|g\|_{H^1},\end{aligned}$$

for some constant $\tilde{C} > 0$ and for all $f, g \in H^1(\mathbb{R}^2)$.

Next we want to show that $\tilde{Q}$ is coercive on $H^1(\mathbb{R}^2)$. We need to show that there exists $\delta > 0$ such that is $|\tilde{Q}(f,f)| \ge \delta\|f\|_{H^1}^2$ for all $f \in H^1(\mathbb{R}^2)$. By Lemma 2.3.1 we see that for all $\varepsilon > 0$ and $f \in H^1(\mathbb{R}^2)$ we have

$$|\tilde{Q}(f,f)| \;\ge\; \frac{1}{2}\|f\|_{H^1}^2 - \frac{1}{2}\|f\|_{L^2}^2 - 3K(\varepsilon\|f\|_{H^1}^2 - \varepsilon^{-1}\|f\|_{L^2}^2) + \lambda\|f\|_{L^2}^2, \tag{2.38}$$

where $K := C \cdot \max\{|\lambda_1|, |\lambda_2|, |\lambda_3|\} > 0$. We can choose λ in the definition of the sesquilinear form $\tilde{Q}$ to be $\lambda := \frac{1}{2} + 3K\varepsilon^{-1} > 0$. Then

$$|\tilde{Q}(f,f)| \ge \frac{1}{2}\|f\|_{H^1}^2 - 3K\varepsilon\|f\|_{H^1}^2 = \left(\frac{1}{2} - 3K\epsilon\right)\|f\|_{H^1}^2, \quad \forall f \in H^1(\mathbb{R}^2), \tag{2.39}$$

which holds for all $\epsilon > 0$. That is we can choose ϵ small enough that $\frac{1}{2} - 3K\epsilon > 0$. Then $\tilde{Q}(f,g)$ is coercive on $H^1(\mathbb{R}^2)$.

We can now apply Theorem 2.2.3 to the sesquilinear form $\tilde{Q}$ and obtain an operator S which is bijective from $D(S)$ onto $L^2(\mathbb{R}^2)$. The operator is given by the relation

$$Q(f,g) = \langle f, Sg\rangle_{L^2}, \quad \forall f \in H^1(\mathbb{R}^2). \tag{2.40}$$

By the properties of the Lebesgue integral we also have that Q is Hermitian, and then by Theorem 2.2.4 the operator S must be self-adjoint. We represent the operator S formally by

$$S = -\frac{1}{2}\frac{\partial^2}{\partial x^2} - \frac{1}{2}\frac{\partial^2}{\partial y^2} + \lambda_1\delta(x) + \lambda_2\delta(y) + \lambda_3\delta(x-y) + \lambda\mathbb{1}, \tag{2.41}$$

where $\lambda_1, \lambda_2, \lambda_3 \in \mathbb{R}$, $\lambda > 0$ and $\mathbb{1}$ is the identity operator.

Note that the operator $H := S - \lambda\mathbb{1}$, for $\lambda \in \mathbb{R}$, is self-adjoint. This is the operator associated with the sesquilinear form in (2.2), and representing the system of interest.

2.4 Domain of the operator

In this section we want to give a detailed description of the domain of the operator H defined in the previous section. For simplicity of notation, it is easier to determine the domain of the operator H associated to the sesquilinear form given by

$$\begin{aligned} Q(f,g) = \iint \overline{\boldsymbol{\nabla} f(x,y)} \cdot \boldsymbol{\nabla} g(x,y)\,\mathrm{d}x\,\mathrm{d}y + \lambda_1 \int \overline{f(x,0)} g(x,0)\,\mathrm{d}x \\ + \lambda_2 \int \overline{f(0,y)} g(0,y)\,\mathrm{d}y + \lambda_3 \int \overline{f(x,x)} g(x,x)\,\mathrm{d}x, \end{aligned} \tag{2.42}$$

where $f, g \in H^1(\mathbb{R}^2)$. The domain of the operator associated to (2.42) is the same as the operator associated to (2.2). We also note that the derivatives of functions in $H^1(\mathbb{R}^2)$ and $H^2(\mathbb{R}^2)$ should be understood in the distributional sense. More on the derivatives of distributions is available in [Reed and Simon, 1980].

By (2.20) and Theorem 2.2.3 the domain of H is defined to be

$$D(H) = \left\{ g \in H^1(\mathbb{R}^2) : \exists C > 0, \forall f \in H^1(\mathbb{R}^2),\ \text{s.t. } |Q(f,g)| \le C\|f\|_{L^2} \right\}. \tag{2.43}$$

We want to give a description of the functions which are in this domain. To do this define the subset $\Omega \subset \mathbb{R}^2$ by

$$\Omega := \{(x,0) \in \mathbb{R}^2 : x \in \mathbb{R}\} \cup \{(0,y) \in \mathbb{R}^2 : y \in \mathbb{R}\} \cup \{(x,x) \in \mathbb{R}^2 : x \in \mathbb{R}\}, \tag{2.44}$$

and the subset $\Omega_m \subset \mathbb{R}^2$ by

$$\begin{aligned} \Omega_m := \{(x,y) \in \mathbb{R}^2 : x \in [-m,m], y \in \mathbb{R}\} \cup \{(x,y) \in \mathbb{R}^2 : y \in [-m,m], x \in \mathbb{R}\} \\ \cup \{(x,y) \in \mathbb{R}^2 : x \in \mathbb{R}, y \in [x-m, x+m]\}, \end{aligned} \tag{2.45}$$

where $m \ge 0$. Similarly, we have the subset $\Omega_m^c := \mathbb{R}^2 \setminus \Omega_m$. This subset is illustrated in Figure 2.1.

Before we prove the first result regarding the domain we need the following lemma.

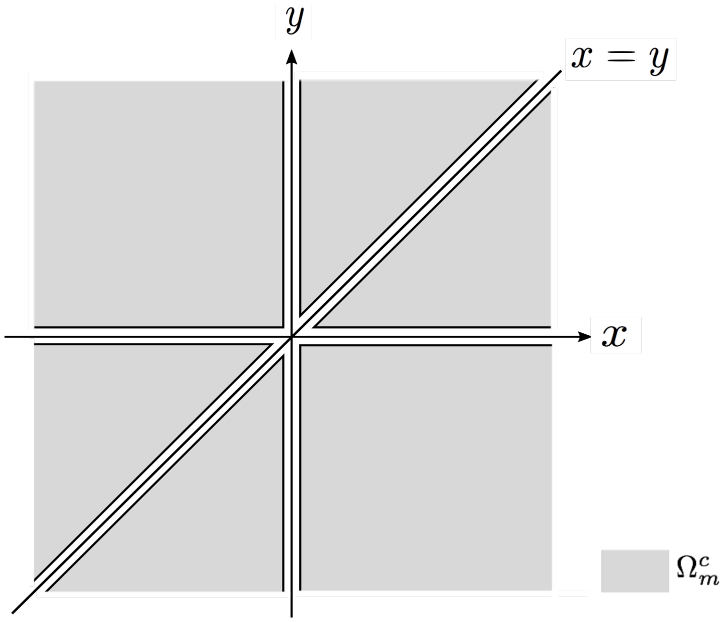

Figure 2.1: Illustration of Ω_m^c

Lemma 2.4.1 *Let $f \in H^1(\mathbb{R}^2)$ and $g \in H^1(\mathbb{R}^2) \cap H^2(\mathbb{R}^2 \setminus \Omega)$. If g satisfies*

$$\lim_{\epsilon \downarrow 0} \int \overline{f(x,0)} \left[\frac{\partial}{\partial y} g(x,-\epsilon) - \frac{\partial}{\partial y} g(x,\epsilon) \right] \, dx = \lambda_1 \int \overline{f(x,0)} g(x,0) \, dx \tag{2.46}$$

$$\lim_{\epsilon \downarrow 0} \int \overline{f(0,y)} \left[\frac{\partial}{\partial x} g(-\epsilon,y) - \frac{\partial}{\partial y} g(\epsilon,y) \right] \, dy = \lambda_2 \int \overline{f(0,y)} g(0,y) \, dy, \tag{2.47}$$

and

$$\lim_{\epsilon \downarrow 0} \int \overline{f(x,x)} \left[\boldsymbol{\nabla} g(x,x-\epsilon) \cdot \boldsymbol{v} - \boldsymbol{\nabla} g(x,x+\epsilon) \cdot \boldsymbol{v} \right] \, dx = \lambda_3 \int \overline{f(x,x)} g(x,x) \, dx, \tag{2.48}$$

where $\boldsymbol{v} = 1/\sqrt{2}(-\boldsymbol{i} + \boldsymbol{j})$ and $\lambda_1, \lambda_2, \lambda_3 \in \mathbb{R}$. Then the following identity holds

$$\int_{\mathbb{R}^2 \setminus \Omega} \overline{\boldsymbol{\nabla} f} \cdot \boldsymbol{\nabla} g \, dx \, dy = - \int_{\mathbb{R}^2 \setminus \Omega} \overline{f} \Delta g \, dx \, dy - \lambda_1 \int \overline{f(x,0)} g(x,0) \, dx - \lambda_2 \int \overline{f(0,y)} g(0,y) \, dy - \lambda_3 \int \overline{f(x,x)} g(x,x) \, dx. \tag{2.49}$$

Proof. Let $f \in H^1(\mathbb{R}^2)$ and $g \in H^2(\mathbb{R}^2 \setminus \Omega)$. To prove the lemma we would like to apply Green's first identity on the left-hand side of (2.49). Green's first identity is given by

$$\int_U \boldsymbol{\nabla} f \cdot \boldsymbol{\nabla} g \, \mathrm{d}x \, \mathrm{d}y = - \int_U f \Delta g \, \mathrm{d}x \, \mathrm{d}y + \oint_{\partial U} f \boldsymbol{\nabla} g \, \mathrm{d}\boldsymbol{v}, \tag{2.50}$$

where $U \subset \mathbb{R}^2$, ∂U is the boundary of U, and $\boldsymbol{v}$ is the unit normal vector of ∂U. The immediate problem with applying this identity to the left-hand side of (2.49) is the restriction of $\boldsymbol{\nabla} g$ to the boundary of $\mathbb{R}^2 \setminus \Omega$. The boundary of $\mathbb{R}^2 \setminus \Omega$ is exactly the lines in Ω. The restriction of $\boldsymbol{\nabla} g$ to these lines is not necessarily defined, since the partial derivatives of g are in $H^1(\mathbb{R}^2 \setminus \Omega)$, and thus we cannot apply Theorem 2.1.1.

Instead, we consider what happens close to the lines in Ω. Let $n \in \mathbb{N}$ and χ_n be the characteristic function given by

$$\chi_n(x,y) := \begin{cases} 1, & \text{if } (x,y) \in \Omega_{1/n}^c \\ 0, & \text{if} (x,y) \in \Omega_{1/n}, \end{cases} \tag{2.51}$$

where $\Omega_{1/n}$ is given by (2.44). By the dominated convergence theorem, p. 26 in [Rudin, 1987], we have

$$\int_{\mathbb{R}^2 \setminus \Omega} \overline{\boldsymbol{\nabla} f} \cdot \boldsymbol{\nabla} g \, \mathrm{d}x \, \mathrm{d}y = \lim_{n \to \infty} \int_{\mathbb{R}^2 \setminus \Omega} \chi_n \overline{\boldsymbol{\nabla} f} \cdot \boldsymbol{\nabla} g \, \mathrm{d}x \, \mathrm{d}y \tag{2.52}$$

$$= \lim_{n \to \infty} \int_{\Omega_{1/n}^c} \overline{\boldsymbol{\nabla} f} \cdot \boldsymbol{\nabla} g \, \mathrm{d}x \, \mathrm{d}y, \tag{2.53}$$

for all $n \in \mathbb{N}$. We are able to apply Green's first identity to the integral in (2.53), since the restriction of $\boldsymbol{\nabla} g$ to the boundaries of $\Omega_{1/n}^c$ is well defined for all $n \in \mathbb{N}$. Green's first identity gives

$$\int_{\Omega_{1/n}^c} \overline{\boldsymbol{\nabla} f} \cdot \boldsymbol{\nabla} g \, \mathrm{d}x \, \mathrm{d}y = - \int_{\Omega_{1/n}^c} \overline{f} \Delta g \, \mathrm{d}x \, \mathrm{d}y + \oint_{\partial \Omega_{1/n}^c} \overline{f} \boldsymbol{\nabla} g \, \mathrm{d}\boldsymbol{v}, \tag{2.54}$$

where $\partial \Omega_{1/n}^c$ is the boundary of the set $\Omega_{1/n}^c$, and $\boldsymbol{v}$ is the outward pointing unit normal vector of $\partial \Omega_{1/n}^c$. From the definition of $\Omega_{1/n}^c$ we see that the second term in (2.54) consist of terms of the type

$$G(x,n) := \int_{1/n}^{\infty} \left[\overline{f(x,-1/n)} \frac{\partial}{\partial y} g(x,-1/n) - \overline{f(x,1/n)} \frac{\partial}{\partial y} g(x,1/n) \right] \mathrm{d}x. \tag{2.55}$$

Rewriting (2.55) and taking the limit as n goes to infinity we get

$$\lim_{n \to \infty} G(x,n) = - \lim_{n \to \infty} \int_{1/n}^{\infty} \overline{f(x,0)} \left[\frac{\partial}{\partial y} g(x,-1/n) - \frac{\partial}{\partial y} g(x,1/n) \right] \mathrm{d}x. \tag{2.56}$$

If we pair all the terms of the final integral on the right-hand side of (2.54) in suitable pairs and take the limit for $n \to \infty$, we can use the dominated convergence theorem and the assumptions in (2.46), (2.47) and (2.48) to find

$$\int_{\mathbb{R}^2 \setminus \Omega} \overline{\boldsymbol{\nabla} f} \cdot \boldsymbol{\nabla} g \, \mathrm{d}x \, \mathrm{d}y = - \int_{\mathbb{R}^2 \setminus \Omega} \overline{f} \Delta g \, \mathrm{d}x \, \mathrm{d}y - \lambda_1 \int \overline{f(x,0)} g(x,0) \, \mathrm{d}x$$
$$- \lambda_2 \int \overline{f(0,y)} g(0,y) \, \mathrm{d}y - \lambda_3 \int \overline{f(x,x)} g(x,x) \, \mathrm{d}x.$$

This concludes the lemma. □

This next result shows that the functions which satisfies the previous lemma are actually in the domain of the operator H.

Theorem 2.4.2 *Let H be the self-adjoint operator associated with* (2.42) *and let $g \in H^1(\mathbb{R}^2) \cap H^2(\mathbb{R}^2 \setminus \Omega)$. Assume furthermore that g satisfies* (2.46),(2.47) *and* (2.48). *Then $g \in D(H)$.*

Proof. Let $f \in H^1(\mathbb{R}^2)$ and let g be as in the theorem. Note that

$$\int_{\mathbb{R}^2} \overline{\nabla f(x,y)} \cdot \nabla g(x,y) \,\mathrm{d}x\,\mathrm{d}y = \int_{\mathbb{R}^2\setminus\Omega} \overline{\nabla f(x,y)} \cdot \nabla g(x,y) \,\mathrm{d}x\,\mathrm{d}y, \tag{2.57}$$

since Ω has Lebesgue measure zero. Applying Lemma 2.4.1, we see that

$$|Q(f,g)| = \left| \int_{\mathbb{R}^2\setminus\Omega} \overline{f(x,y)} \Delta g(x,y) \,\mathrm{d}x\,\mathrm{d}y \right| \tag{2.58}$$

$$\leq \|\Delta g\|_{L^2(\mathbb{R}^2\setminus\Omega)} \|f\|_{L^2(\mathbb{R}^2\setminus\Omega)} = C\|f\|_{L^2(\mathbb{R}^2)}, \tag{2.59}$$

then $g \in D(H)$ by (2.43). □

The inclusion of the functions satisfying Lemma 2.4.1 in $D(H)$ have now been shown. We want to show that the opposite inclusion holds aswell. Proving this inclusion is somewhat more difficult. We will define a family of functions $\phi_{m,M} \in C^\infty(\mathbb{R}^2)$, where $0 \leq \phi_{m,M}(\boldsymbol{x}) \leq 1$ for all $\boldsymbol{x} \in \mathbb{R}^2$, as

$$\phi_{m,M}(\boldsymbol{x}) = \begin{cases} 0, & \boldsymbol{x} \in \Omega_m \\ 1, & \boldsymbol{x} \in \Omega_M^c, \end{cases} \tag{2.60}$$

where $0 \leq m < M$. That such a family of functions actually do exist is something that should be proven. But we will skip that proof, because it does not fit the scope of the project.

To prove the opposite inclusion we need the following two lemmas.

Lemma 2.4.3 *Let Q be the sesquilinear form given by* (2.42), *and H be the self-adjoint operator associated with Q. If $f \in D(H)$ and $\phi_{m,M} \in C^\infty(\mathbb{R}^2)$, where $0 \leq m < M$. Then $f\phi_{m,M} \in H^2(\mathbb{R}^2)$.*

Proof. We denote $\phi_{m,M}$ by ϕ. By the definition of Sobolev spaces and Plancherel's theorem we just need to show that $\Delta(f\phi) \in L^2(\mathbb{R}^2)$. Let $\psi \in \mathcal{D}(\mathbb{R}^2)$, the set of test-functions defined on p. 148 in [Reed and Simon, 1980]. Then by the definition of the distributional derivative, we have

$$\langle\psi, \Delta(f\phi)\rangle = -\langle\boldsymbol{\nabla}\psi, \boldsymbol{\nabla}(f\phi)\rangle \tag{2.61}$$
$$= -\langle\boldsymbol{\nabla}\psi, f\boldsymbol{\nabla}\phi + \phi\boldsymbol{\nabla}f\rangle \tag{2.62}$$
$$= -\langle\boldsymbol{\nabla}\psi, f\boldsymbol{\nabla}\phi\rangle - \langle\boldsymbol{\nabla}\psi, \phi\boldsymbol{\nabla}f\rangle \tag{2.63}$$
$$= -\langle\boldsymbol{\nabla}\psi, f\boldsymbol{\nabla}\phi\rangle - \langle\phi\boldsymbol{\nabla}\psi, \boldsymbol{\nabla}f\rangle \tag{2.64}$$
$$= -\langle\boldsymbol{\nabla}\psi, f\boldsymbol{\nabla}\phi\rangle + \langle\psi\boldsymbol{\nabla}\phi, \boldsymbol{\nabla}f\rangle - \langle\boldsymbol{\nabla}(\psi\phi), \boldsymbol{\nabla}f\rangle \tag{2.65}$$
$$= \langle\psi, \boldsymbol{\nabla}\cdot(f\boldsymbol{\nabla}\phi)\rangle + \langle\psi\boldsymbol{\nabla}\phi, \boldsymbol{\nabla}f\rangle - \langle\boldsymbol{\nabla}(\psi\phi), \boldsymbol{\nabla}f\rangle. \tag{2.66}$$

But by the definition of ϕ we have that

$$\lambda_1 \int \overline{(\psi\phi)(x,0)} f(x,0)\,\mathrm{d}x = 0 \tag{2.67}$$
$$\lambda_2 \int \overline{(\psi\phi)(0,y)} f(0,y)\,\mathrm{d}y = 0 \tag{2.68}$$
$$\lambda_3 \int \overline{(\psi\phi)(x,x)} f(x,x)\,\mathrm{d}x = 0, \tag{2.69}$$

Then the definition of Q and (2.66) implies that

$$\langle\psi, \Delta(f\phi)\rangle = \langle\psi, \boldsymbol{\nabla}\cdot(f\boldsymbol{\nabla}\phi)\rangle + \langle\psi\boldsymbol{\nabla}\phi, \boldsymbol{\nabla}f\rangle - Q(\psi\phi, f). \tag{2.70}$$

Since $f \in D(H)$ we find

$$\langle\psi, \Delta(f\phi)\rangle = \langle\psi, \boldsymbol{\nabla}\cdot(f\boldsymbol{\nabla}\phi)\rangle + \langle\psi, (\boldsymbol{\nabla}\phi)\cdot(\boldsymbol{\nabla}f)\rangle) - \langle\psi, \phi Hf\rangle. \tag{2.71}$$

This holds for all $\psi \in \mathcal{D}(\mathbb{R}^2)$, so we must have

$$\Delta(f\phi) = \boldsymbol{\nabla}\cdot(f\boldsymbol{\nabla}\phi) + (\boldsymbol{\nabla}\phi)\cdot(\boldsymbol{\nabla}f) - \phi Hf \tag{2.72}$$
$$= f\Delta\phi + 2(\boldsymbol{\nabla}\phi)\cdot(\boldsymbol{\nabla}f) - \phi Hf. \tag{2.73}$$

By the definition of ϕ we know that $\Delta\phi$ is bounded, which implies that $f\Delta\phi \in L^2(\mathbb{R}^2)$. Furthermore $\boldsymbol{\nabla}\phi\cdot\boldsymbol{\nabla}f \in L^2(\mathbb{R}^2)$, since $f \in H^1(\mathbb{R}^2)$ and the partial derivatives of ϕ are bounded. Finally, since $f \in D(H)$ and $H : D(H) \to L^2(R^2)$ we know that $Hf \in L^2(\mathbb{R}^2)$ and consequently $\phi Hf \in L^2(\mathbb{R}^2)$. This shows that $\Delta(f\phi) \in L^2(\mathbb{R}^2)$. □

Lemma 2.4.4 *Let $f \in H^1(\mathbb{R}^2)$. Then $f \in H^1(\mathbb{R}^2)\cap H^2(\mathbb{R}^2\setminus\Omega)$, where Ω is given by* (2.44)*, if and only if $\phi_{m,M}\Delta f \in L^2(\mathbb{R}^2)$, and*

$$\lim_{M\downarrow 0} \int |\phi_{m,M}\Delta f(\boldsymbol{x})|^2\, d\boldsymbol{x} < \infty, \tag{2.74}$$

for all $0 \le m < M$.

Proof. Assume that $f \in H^1(\mathbb{R}^2) \cap H^2(\mathbb{R}^2 \setminus \Omega)$. Then $\Delta f \in L^2(\mathbb{R}^2 \setminus \Omega)$ by Plancherel's theorem and the definition of Sobolev spaces. This implies that $\phi_{m,M}\Delta f \in L^2(\mathbb{R}^2)$ for all $0 \leq m < M$. Additionally, we know

$$|\phi_{m,M}\Delta f(\boldsymbol{x})| \leq |\Delta f(\boldsymbol{x})|, \tag{2.75}$$

for all $0 \leq m < M$ and $\boldsymbol{x} \in \mathbb{R}^2 \setminus \Omega$. Furthermore, $\phi_{m,M}\Delta f(\boldsymbol{x}) \to \Delta f(\boldsymbol{x})$ for $M \searrow 0$. Then by the dominated convergence theorem

$$\lim_{M\downarrow 0} \int_{\mathbb{R}^2} |\phi_{m,M}\Delta f(\boldsymbol{x})|^2 \, \mathrm{d}\boldsymbol{x} = \int_{\mathbb{R}^2\setminus\Omega} |\Delta f(\boldsymbol{x})|^2 \, \mathrm{d}\boldsymbol{x} < \infty. \tag{2.76}$$

This concludes the first part of the proof.

Assume conversely that $\phi_{m,M}\Delta f \in L^2(\mathbb{R}^2)$ and that (2.74) holds for all $0 \leq m < M$. Then by the dominated convergence theorem

$$\int_{\mathbb{R}^2\setminus\Omega} |\Delta f(\boldsymbol{x})|^2 \, \mathrm{d}\boldsymbol{x} = \lim_{M\downarrow 0} \int_{\mathbb{R}^2} |\phi_{m,M}\Delta f(\boldsymbol{x})|^2 \, \mathrm{d}\boldsymbol{x} < \infty. \tag{2.77}$$

Then $\Delta f \in L^2(\mathbb{R}^2 \setminus \Omega)$, and consequently, $f \in H^1(\mathbb{R}^2) \cap H^2(\mathbb{R}^2 \setminus \Omega)$. □

We are now ready to prove the first part of the inclusion. We begin by showing that if $f \in D(H)$, then $f \in H^1(\mathbb{R}^2) \cap H^2(\mathbb{R}^2 \setminus \Omega)$.

Theorem 2.4.5 *Let Q be the sesquilinear form given by* (2.42)*, and H be the self-adjoint operator associated with Q. If $f \in D(H)$, then $f \in H^1(\mathbb{R}^2) \cap H^2(\mathbb{R}^2 \setminus \Omega)$.*

Proof. Assume that $f \in D(H)$. We then want to show that f satisfies the conditions in Lemma 2.4.4. Obviously $f \in H^1(\mathbb{R}^2)$.

We begin by showing that $\phi_{m,M}\Delta \in L^2(\mathbb{R}^2)$ for all $0 \leq m < M$. By Lemma 2.4.3 we know that $\Delta(\phi_{m,M} f) \in L^2(\mathbb{R}^2)$, for all $0 \leq m < M$. Let $\psi \in \mathcal{D}(\mathbb{R}^2)$, then

$$\langle \psi, \Delta(\phi_{m,M} f)\rangle = \langle \psi, \phi_{m,M}\Delta f + 2\boldsymbol{\nabla} f \cdot \boldsymbol{\nabla}\phi_{m,M} + f\Delta\phi_{m,M}\rangle. \tag{2.78}$$

Since ψ was arbitrary we have

$$\Delta(\phi_{m,M} f) = \phi_{m,M}\Delta f + 2\boldsymbol{\nabla} f \cdot \boldsymbol{\nabla}\phi_{m,M} + f\Delta\phi_{m,M}. \tag{2.79}$$

But $\boldsymbol{\nabla} f \cdot \boldsymbol{\nabla}\phi_{m,M} \in L^2(\mathbb{R}^2)$ and $f\Delta\phi_{m,M} \in L^2(\mathbb{R}^2)$. Then $\phi_{m,M}\Delta f \in L^2(\mathbb{R}^2)$, for all $0 \leq m < M$. Note also that by (2.79) and (2.73) we have

$$\phi_{m,M}\Delta f = -\phi_{m,M} H f. \tag{2.80}$$

We now need to show that (2.74) holds. But using (2.80) we have

$$\lim_{M\downarrow 0} \int |\phi_{m,M}\Delta f|^2 \, \mathrm{d}x = \lim_{M\downarrow 0} \int |\phi_{m,M} H f|^2 \, \mathrm{d}x \tag{2.81}$$

$$\leq \int |Hf|^2 \, \mathrm{d}x < \infty, \tag{2.82}$$

for all $0 \leq m < M$, since $Hf \in L^2(\mathbb{R}^2)$. Applying Lemma 2.4.4 concludes the proof. $\square$

Finally, it only remains to show that if $g \in D(H)$, then (2.46), (2.47) and (2.48) holds.

Theorem 2.4.6 *Let Q be the sesquilinear form given by* (2.42)*, and H be the self-adjoint operator associated with Q. If $g \in D(H)$, then* (2.46)*,* (2.47) *and* (2.48) *holds.*

Proof. Let $g \in D(H)$ and $f \in H^1(\mathbb{R}^2)$. We write $Q(f,g)$ as

$$Q(f,g) = \int_{\mathbb{R}^2} \overline{\boldsymbol{\nabla} f} \cdot \boldsymbol{\nabla} g \,\mathrm{d}x\,\mathrm{d}y + \tilde{Q}(f,g), \tag{2.83}$$

where

$$\tilde{Q}(f,g) = \int_{\mathbb{R}} \overline{f(x,0)} g(x,0)\,\mathrm{d}x + \int_{\mathbb{R}} \overline{f(0,y)} g(0,y)\,\mathrm{d}y + \int_{\mathbb{R}} \overline{f(x,x)} g(x,x)\,\mathrm{d}x. \tag{2.84}$$

We can then split the first integral in (2.83) into two integrals, and write

$$Q(f,g) = \int_{\Omega_M^{\perp}} \overline{\boldsymbol{\nabla} f} \cdot \boldsymbol{\nabla} g \,\mathrm{d}x\,\mathrm{d}y + \int_{\Omega_M} \overline{\boldsymbol{\nabla} f} \cdot \boldsymbol{\nabla} g \,\mathrm{d}x\,\mathrm{d}y + \tilde{Q}(f,g), \tag{2.85}$$

where $M > 0$ and Ω_M is given by (2.45). We use Greens first identity on the first integral in (2.85) to obtain

$$\int_{\Omega_M^{\perp}} \overline{\boldsymbol{\nabla} f} \cdot \boldsymbol{\nabla} g \,\mathrm{d}x\,\mathrm{d}y = -\int_{\Omega_M^{\perp}} \overline{f} \Delta g \,\mathrm{d}x\,\mathrm{d}y + \oint_{\partial\Omega_M^{\perp}} \overline{f} \boldsymbol{\nabla} g \cdot \,\mathrm{d}\boldsymbol{v}. \tag{2.86}$$

But $\phi_{m,M}$ is identical one on $\Omega_M^{\perp}$ by the definition of $\phi_{m,M}$, then we can write

$$-\int_{\Omega_M^{\perp}} \overline{f} \Delta g \,\mathrm{d}x\,\mathrm{d}y = -\int_{\Omega_M^{\perp}} \overline{f} \phi_{m,M} \Delta g \,\mathrm{d}x\,\mathrm{d}y. \tag{2.87}$$

We also have that $-\phi_{m,M}\Delta g = \phi_{m,M} H g$ by (2.80). If we take the limit when $M \to 0$ of (2.87) and use the dominated convergence theorem, we find that

$$\lim_{M \to 0} \int_{\Omega_M^{\perp}} \overline{f} \phi_{m,M} H g \,\mathrm{d}x\,\mathrm{d}y = \langle f, Hg \rangle = Q(f,g). \tag{2.88}$$

The equations (2.85), (2.86) and (2.88) imply that

$$\lim_{M \to 0} \left\{ \tilde{Q}(f,g) + \oint_{\partial\Omega_M^{\perp}} \overline{f} \boldsymbol{\nabla} g \cdot \,\mathrm{d}\boldsymbol{v} + \int_{\Omega_M} \overline{\boldsymbol{\nabla} f} \cdot \boldsymbol{\nabla} g \,\mathrm{d}x\,\mathrm{d}y \right\} = 0. \tag{2.89}$$

The limit when $M \to 0$ of the last integral in (2.89) is zero, since it is becomes the integral over a set of measure zero. Finally we get the relation

$$\lim_{M \to 0} \left\{ \tilde{Q}(f,g) + \oint_{\partial\Omega_M^{\perp}} \overline{f} \boldsymbol{\nabla} g \cdot \,\mathrm{d}\boldsymbol{v} \right\} = 0. \tag{2.90}$$

Writing the contributions of the integral explicitly we see that the theorem holds. $\square$

Theorem 2.4.7 *Let Q be the sesquilinear form given by* (2.42) *and H the self-adjoint operator associated with Q. Then the domain of $D(H)$ given by* (2.43) *is equal to*

$$S := \left\{ f \in H^1(\mathbb{R}^2) : f \in H^2(\mathbb{R}^2 \setminus \Omega), \ \textit{and } (2.46), (2.47), (2.48) \textit{ holds.} \right\}, \quad (2.91)$$

where Ω is given by (2.44).

Proof. The inclusion $D(H) \subseteq S$ is proven in Theorem 2.4.2. The inclusion $S \subseteq D(H)$ is proved in Theorems 2.4.5 and 2.4.6 □

The precise description of the domain of H is now done, and we can move on to the spectral analysis of the system.

Chapter 3

Essential Spectrum of the Operator

In this chapter, we want to determine the essential spectrum of the operator we constructed in the previous chapter. The essential spectrum of an operator is defined in Definition A.2.6. Let us denote H by

$$H_{\lambda_1\lambda_2\lambda_3} = -\frac{1}{2}\frac{\partial^2}{\partial x^2} - \frac{1}{2}\frac{\partial^2}{\partial y^2} + \lambda_1\delta(x) + \lambda_2\delta(y) + \lambda_3\delta(x-y). \tag{3.1}$$

In this chapter we assume that $\lambda_1, \lambda_2 < 0$, and $\lambda_3 > 0$. This can be interpreted as a one-dimensional system consisting of a positively charged nucleus with infinite mass, and two electrons with mass equal to one.

The main result in this chapter is a special case of the Hunziker - van Winter - Zhislin theorem, usually called the HVZ theorem. The HVZ theorem will give us the essential spectrum of $H_{\lambda_1\lambda_2\lambda_3}$. To prove the HVZ theorem we need various results, which will be presented in the following sections.

3.1 Weyl's Criterion and Weyl Sequences

In this section, we present Weyl sequences and Weyl's criterion. Weyl's criterion gives a sufficient condition for $\lambda \in \mathbb{R}$ to be in the essential spectrum of a self-adjoint operator. But we begin by defining Weyl sequences.

Definition 3.1.1
Let A be a self-adjoint operator. A sequence $\{\psi_n\} \subset D(A)$ is called a Weyl sequence for A and $\lambda \in \mathbb{C}$ if it satisfies

1. $\|\psi_n\| = 1$
2. $\|(A-\lambda)\psi_n\| \to 0$ *for* $n \to \infty$

3. *ψ_n converges weakly to zero.*

We note that if $\{\psi_n\}$ converges weakly to zero, then it is an orthogonal sequence. Next we state Weyl's criterion.

Theorem 3.1.2 (Weyl's Criterion) *Let A be a self-adjoint operator. Then $\lambda \in \sigma_{ess}(A)$ if and only if there exists a Weyl sequence for A and λ.*

Proof. For a proof see Section 7.2 and 7.3 in [Hislop and Sigal, 1996]. □

We want to determine the spectrum and find a Weyl sequences for the operator $-\Delta$ on $H^2(\mathbb{R}^d)$. The construction of the Weyl sequences is contained in the proof of the next theorem. Note that we have not proved that $-\Delta$ is actually a self-adjoint operator on $H^2(\mathbb{R}^d)$, but we refer to Example 8.4 in [Hislop and Sigal, 1996] for the proof.

Theorem 3.1.3 *The spectrum of the self-adjoint operator $-\Delta$ on $H^2(\mathbb{R}^d)$ is $\sigma(-\Delta) = \sigma_{ess}(-\Delta) = [0, \infty)$.*

Proof. For simplicity of notation, we will only prove the theorem for $d = 1$. Let $\psi \in D(-\Delta) = H^2(\mathbb{R})$, then

$$\langle \psi, -\Delta\psi \rangle = \int k^2 |\hat{\psi}(k)|^2 \, \mathrm{d}k \geq 0. \tag{3.2}$$

This shows that $-\Delta$ is a positive operator on $H^2(\mathbb{R})$. Then $\sigma(-\Delta) \subseteq [0, \infty)$. We then use Weyl's criterion to show that if $\lambda > 0$ then $\lambda \in \sigma_{ess}(-\Delta)$. That is, we need to construct a Weyl sequence for λ and $-\Delta$. Consider the function $\phi \in C_0^\infty(\mathbb{R})$, with

$$\phi(x) = \begin{cases} 1, & \text{if } |x| \leq 1/4 \\ 0, & \text{if } |x| \geq 1/2, \end{cases} \tag{3.3}$$

and $0 \leq \phi(x) \leq 1$ for all $x \in \mathbb{R}$. Define the sequence $\{\phi_n\}$ by $\phi_n(x) := \phi(x/n - n)$. Let $\lambda > 0$ and let $\{j_{n,\lambda}\}$ be the sequence defined by

$$j_{n,\lambda}(x) = \frac{\phi_n(x)}{\sqrt{n}\|\phi\|} e^{i\sqrt{\lambda}x}. \tag{3.4}$$

This sequence is shown to be a Weyl sequence for λ and $-\Delta$. It is obviously in $H^2(\mathbb{R})$ since $\phi_n \in C_0^\infty(\mathbb{R})$. It is normalized since

$$\|j_{n,\lambda}\|^2 = \frac{1}{n\|\phi\|^2} \int |\phi(x/n - n)|^2 \, \mathrm{d}x \tag{3.5}$$

$$= \frac{1}{n\|\phi\|^2} \int |\phi(x/n)|^2 \, \mathrm{d}x \tag{3.6}$$

$$= \frac{1}{\|\phi\|^2} \int |\phi(t)|^2 \, \mathrm{d}x = 1. \tag{3.7}$$

Next we show that the sequence $\{j_{n,\lambda}\}$ converges weakly to zero. For $\varphi \in L^2(\mathbb{R})$ consider

$$|\langle \varphi, j_{n,\lambda}\rangle|^2 \leq \frac{1}{n\|\phi\|^2} \int |\varphi(x)\phi_n(x)|^2 \,\mathrm{d}x \tag{3.8}$$

$$\leq \frac{1}{n\|\phi\|^2} \int |\varphi(x)|^2 \,\mathrm{d}x \tag{3.9}$$

$$\leq \frac{C}{n}, \tag{3.10}$$

for some constant $C > 0$ and $n \in \mathbb{N}$. It follows that $|\langle \varphi, \psi_n\rangle|^2 \to 0$ for $n \to \infty$, and specifically $\langle \varphi, \psi_n\rangle \to 0$ for $n \to \infty$. Then $\{j_{n,\lambda}\}$ converges weakly to zero on $H^2(\mathbb{R})$. Consider

$$\|(-\Delta - \lambda) j_{n,\lambda}\|^2 \leq \frac{1}{n\|\phi\|^2} \left(\|\phi_n''\|^2 + 2\sqrt{\lambda}\|\phi_n'\|^2\right) \tag{3.11}$$

$$\leq \frac{C}{n^2}, \tag{3.12}$$

for some $C > 0$. Then $\|(-\Delta - \lambda) j_{n,\lambda}\| \to 0$ for $n \to \infty$.

We have now shown that $(0, \infty) \subseteq \sigma_{ess}(-\Delta)$. Since the spectrum is a closed set we have that $[0, \infty) \subseteq \sigma(-\Delta)$, and consequently $\sigma(-\Delta) = [0, \infty)$. Finally, zero is not an isolated eigenvalue, and hence $\sigma(-\Delta) = \sigma_{ess}(-\Delta) = [0, \infty)$. □

We use the constructed Weyl sequence for $-\Delta$ on $H^2(\mathbb{R}^d)$ in the proof of the HVZ theorem in Section 3.4. Additionally, we use that $\sigma(-\Delta) = [0, \infty)$ many times in the later chapters. In the next section we present the Helffer-Sjöstrand formula, which is another result we use to prove the HVZ theorem.

3.2 The Helffer-Sjöstrand Formula

The main result of this section is Helffer-Sjöstrand's formula. Before we can prove the formula, we need to consider a special type of functions called almost analytical functions. Recall that a function $f(z) = u(x, y) + iv(x, y)$, for $z = x + iy$ is an analytic function if and only if it satisfies the Cauchy-Riemann equations

$$\frac{\partial u}{\partial x} = \frac{\partial v}{\partial y}, \quad \text{and} \quad \frac{\partial u}{\partial y} = -\frac{\partial v}{\partial x}. \tag{3.13}$$

We can define the differential operator $\overline{\partial}$ as

$$\overline{\partial} := \frac{1}{2}\left(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y}\right), \tag{3.14}$$

and note that for an analytic function $f(z)$, we have $\overline{\partial} f(z) = 0$.

We now introduce the functions called "almost" analytic functions. Let $f \in C_0^\infty(\mathbb{R})$ where f has support in the interval $[a,b]$, and $f(a) = f(b) = 0$. Define $\tilde{f}(z)$, an extension of $f(x)$ to the complex plane, as

$$\tilde{f}(z) := \left(f(x) + f'(x)iy + \frac{f''(x)}{2!}(iy)^2 + \cdots + \frac{f^{(n)}(x)}{n!}(iy)^n \right) g(y) \tag{3.15}$$

$$= g(y) \sum_{j=0}^{n} \frac{f^{(j)}(x)}{j!}(iy)^j, \tag{3.16}$$

where $z = x + iy$, and n is some integer satisfying $n \geq 1$, and $g(y) \in C_0^\infty$ is a function satisfying g

$$g(y) = \begin{cases} 1, & |y| \leq \frac{1}{4}, \\ 0, & |y| > \frac{1}{2}. \end{cases} \tag{3.17}$$

We see that $\overline{\partial}\tilde{f}$ is given by

$$\overline{\partial}\tilde{f} = g(y) \left(\sum_{j=0}^{n} \frac{f^{(j+1)}(x)}{j!}(iy)^j \right) + i \left(g'(y)\frac{\tilde{f}(z)}{g(y)} + ig(y) \sum_{j=1}^{n} \frac{f^{(j)}(x)}{(j-1)!}(iy)^{j-1} \right)$$

$$= ig'(y)\frac{\tilde{f}(z)}{g(y)} + g(y)\frac{f^{(n+1)}(x)}{n!}(iy)^n. \tag{3.18}$$

For $y \to 0$, the behavior of $|\overline{\partial}\tilde{f}(z)|$ is $\mathcal{O}(|y|^n)$. Additionally, $\overline{\partial}\tilde{f}(z) = 0$ holds for $z \in \mathbb{R}$, which is why $\tilde{f}$ is called an almost analytic function. We use this type of function to prove the Helffer-Sjöstrand formula.

Theorem 3.2.1 (Helffer-Sjöstrand Formula) *Let A be a self-adjoint operator on a Hilbert space $\mathcal{A}$. Suppose $f \in C_0^\infty(\mathbb{R})$ with support in $[a,b]$ and $f(a) = f(b) = 0$. Let $\tilde{f}(z)$ be the almost analytic extension defined by* (3.15)*. Then we can write*

$$f(A) = -\frac{1}{\pi} \int_\Omega \overline{\partial}\tilde{f}(z)(A-z)^{-1}\, dy\, dx, \tag{3.19}$$

where $\Omega = [a,b] \times [-1,1]$.

Proof. Let $f \in C_0^\infty(\mathbb{R})$ be as in the theorem. By the special case of Stone's formula in (A.18) we can write $f(A)$ as

$$f(A) = \frac{1}{2\pi i} \operatorname*{s-lim}_{\varepsilon \downarrow 0} \int_a^b f(x) \left[R_A(x - i\varepsilon) - R_A(x + i\varepsilon) \right] \mathrm{d}x. \tag{3.20}$$

So we need to show that (3.20) and (3.19) are equal. To show this, we evaluate the integrand in (3.19). Consider

$$\overline{\partial}\left(\tilde{f}(z)(A-z)^{-1}\right) = (A-z)^{-1}\overline{\partial}\tilde{f}(z) + \tilde{f}(z)\overline{\partial}(A-z)^{-1}. \tag{3.21}$$

From the first resolvent equation, (A.6), it is possible to show that $(A-z)^{-1}$ is analytic on the resolvent set. Consequently,

$$\overline{\partial}\left(\tilde{f}(z)(A-z)^{-1}\right) = (A-z)^{-1}\overline{\partial}\tilde{f}(z), \tag{3.22}$$

by the Cauchy-Riemann equations. Let $F(x,y) := \tilde{f}(z)(A-z)^{-1}$, where $z = x+iy$, then (3.19) can be written as

$$f(A) = -\frac{1}{\pi}\operatorname*{s-lim}_{\varepsilon\downarrow 0}\left(\int_a^b\int_{-1}^{-\varepsilon}\overline{\partial}F(x,y)\,\mathrm{d}y\,\mathrm{d}x + \int_a^b\int_{\varepsilon}^{1}\overline{\partial}F(x,y)\,\mathrm{d}y\,\mathrm{d}x\right). \tag{3.23}$$

We consider the first term. By the fundamental theorem of calculus, and the fact that $f(a) = f(b) = 0$ and $g(1) = g(-1) = 0$, we can write the first term of (3.23) as

$$\begin{aligned}\int_a^b\int_{-1}^{-\varepsilon}\overline{\partial}F(x,y)\,\mathrm{d}y\,\mathrm{d}x &= \frac{1}{2}\int_a^b\int_{-1}^{-\varepsilon}\left(\frac{\partial}{\partial x}F(x,y) + i\frac{\partial}{\partial y}F(x,y)\right)\,\mathrm{d}y\,\mathrm{d}x\\ &= \frac{i}{2}\int_a^b F(x,-\varepsilon)\,\mathrm{d}x. \end{aligned}\tag{3.24}$$

Similar calculations can be done for the second term of (3.23). We get that

$$\begin{aligned}f(A) &= -\frac{i}{2\pi}\operatorname*{s-lim}_{\varepsilon\downarrow 0}\int_a^b\left(F(x,-\varepsilon) - F(x,\varepsilon)\right)\,\mathrm{d}x \qquad (3.25)\\ &= \frac{1}{2\pi i}\operatorname*{s-lim}_{\varepsilon\downarrow 0}\int_a^b\left(\tilde{f}(x-i\varepsilon)R_A(x-i\varepsilon) - \tilde{f}(x+i\varepsilon)R_A(x+i\varepsilon)\right)\,\mathrm{d}x.\end{aligned}$$

To finish the proof, we examine what happens when $\varepsilon \to 0$. By Theorem A.2.3 we have

$$\|R_A(x+i\varepsilon)\| \le |\varepsilon|^{-1}, \quad \text{and} \quad \|R_A(x-i\varepsilon)\| \le |\varepsilon|^{-1}. \tag{3.26}$$

The singularity which arises by (3.26) is cancelled for the terms of $\tilde{f}(z)$, which are proportional to at least $|y|^2$. By the definition of $\tilde{f}(z)$ in (3.15) only the first and the second terms survive. We get that

$$\begin{aligned}f(A) = -\frac{1}{2\pi i}\operatorname*{s-lim}_{\varepsilon\downarrow 0}\Bigg[&\int_a^b f(x)\left[R_A(x-i\varepsilon) - R_A(x+i\varepsilon)\right]\,\mathrm{d}x\\ &+ i\varepsilon\int_a^b f'(x)\left[R_A(x-i\varepsilon) + R_A(x+i\varepsilon)\right]\,\mathrm{d}x\Bigg].\end{aligned}\tag{3.27}$$

To finish the proof we just need to show that the second term in (3.27) goes to zero when ε goes to zero. To see this, note that by the Spectral Theorem we can write

$$g(A) = \int g(\lambda)\,\mathrm{d}P_A(\lambda). \tag{3.28}$$

Let $g(A)$ be given by

$$g(A) := \varepsilon\int_a^b f'(x)\left[R_A(x-i\varepsilon) + R_A(x+i\varepsilon)\right]\,\mathrm{d}x. \tag{3.29}$$

Integration by parts gives

$$g(A) = \varepsilon \iint_a^b f'(x) \left[\frac{1}{\lambda - x + i\varepsilon} + \frac{1}{\lambda - x - i\varepsilon} \right] \mathrm{d}x \, \mathrm{d}P_A(\lambda) \tag{3.30}$$

$$= \varepsilon \iint_a^b \frac{2f'(x)(\lambda - x)}{(\lambda - x)^2 + \varepsilon^2} \mathrm{d}x \, \mathrm{d}P_A(\lambda) \tag{3.31}$$

$$= -2\varepsilon \iint_a^b (f''(x)(\lambda - x) - f'(x)) \log[(\lambda - x)^2 + \varepsilon^2] \, \mathrm{d}x \, \mathrm{d}P_A(\lambda)$$

By the dominated convergence theorem, and since the logarithm is integrable over a singularity, we have that $g(A)$ goes to zero for $\varepsilon \to 0$. □

3.3 The operators $f(-i\Delta)$ and $g(\cdot)f(-i\Delta)$

In this section we present two lemmas which are needed to prove the HVZ theorem. In this section we will sometimes use $\mathscr{F}$ and $\mathscr{F}^{-1}$ for the Fourier transform and the inverse Fourier transform, since it is a useful notation for this section. More information on the type of operators we work with in this section is available in [Simon, 2005].

Recall that if Δ is the Laplacian, we can write

$$-\Delta = \mathscr{F}^{-1} k^2 \mathscr{F}. \tag{3.32}$$

Similarly if $f : \mathbb{R}^d \to \mathbb{R}$ is a bounded an measurable function, we can write

$$f(-\Delta) = \mathscr{F}^{-1} f(k^2) \mathscr{F}. \tag{3.33}$$

This motivates us to define the operator $f(-i\boldsymbol{\nabla})$, for $f \in L^\infty(\mathbb{R}^d)$, on $\psi \in L^2(\mathbb{R}^d)$ as

$$[f(-i\boldsymbol{\nabla})\psi](\boldsymbol{x}) := \widecheck{f(\boldsymbol{k})\hat{\psi}(\boldsymbol{k})}(\boldsymbol{x}) = \frac{1}{(2\pi)^{d/2}} \int \check{f}(\boldsymbol{x} - \boldsymbol{y}) \psi(\boldsymbol{y}) \, \mathrm{d}\boldsymbol{y}. \tag{3.34}$$

Similarly, let $g \in L^2(\mathbb{R}^d) \cap L^\infty(\mathbb{R}^d)$. Then the operator $g(\cdot)f(-i\boldsymbol{\nabla})$ is defined as the integral operator with kernel given by

$$[g(\cdot)f(-i\boldsymbol{\nabla})](\boldsymbol{x}, \boldsymbol{y}) = \frac{1}{(2\pi)^{d/2}} g(\boldsymbol{x}) \check{f}(\boldsymbol{x} - \boldsymbol{y}). \tag{3.35}$$

In the next result we show that for f belonging to a certain class of functions this operator is compact.

Lemma 3.3.1 *Let $g \in L^2(\mathbb{R}^d) \cap L^\infty(\mathbb{R}^d)$ and $f \in L^\infty(\mathbb{R}^d)$. If $f(\boldsymbol{k}) \to 0$ for $|\boldsymbol{k}| \to \infty$, then the operator $g(\cdot)f(-i\boldsymbol{\nabla})$ is compact.*

Proof. We prove the lemma by constructing a sequence of Hilbert-Schmidt operators which is norm convergent to $g(\cdot)f(-i\boldsymbol{\nabla})$. Let $\phi \in C_0^\infty(\mathbb{R}^d)$ be a function which satisfies $0 \le \phi(\boldsymbol{k}) \le 1$ for all $\boldsymbol{k} \in \mathbb{R}^d$, and

$$\phi(\boldsymbol{k}) = \begin{cases} 1, & \text{if } |\boldsymbol{k}| \le 1, \\ 0, & \text{if } |\boldsymbol{k}| \ge 2. \end{cases} \tag{3.36}$$

Define $\phi_n(\boldsymbol{k}) := \phi(\boldsymbol{k}/n)$, where $n \in \mathbb{N}$. Then a sequence of operators can be defined by

$$T_n := g(\cdot)[\phi_n f](-i\boldsymbol{\nabla}). \tag{3.37}$$

We show that T_n is Hilbert-Schmidt for all $n \in \mathbb{N}$. The Hilbert-Schmidt norm of T_n is

$$\|T_n\|_{HS}^2 = \frac{1}{(2\pi)^d} \iint |g(\boldsymbol{x})|^2 |\widecheck{\phi_n f}(\boldsymbol{y}-\boldsymbol{x})|^2 \, \mathrm{d}\boldsymbol{x} \, \mathrm{d}\boldsymbol{y} \tag{3.38}$$

$$= \frac{1}{(2\pi)^d} \int |g(\boldsymbol{x})|^2 \left(\int |\widecheck{\phi_n f}(\boldsymbol{y}-\boldsymbol{x})|^2 \, \mathrm{d}\boldsymbol{y} \right) \mathrm{d}\boldsymbol{x}. \tag{3.39}$$

The final equality is due to Fubini's theorem. Since $\phi_n f$ is a bounded function with compact support we have $\phi_n f \in L^2(\mathbb{R}^d)$ for all $n \in \mathbb{N}$. Then by Plancherel's theorem we have

$$\|T_n\|_{HS}^2 = \frac{1}{(2\pi)^d} \|\phi_n f\|_{L^2}^2 \|g\|_{L^2}^2 < \infty. \tag{3.40}$$

Consequently, $\{T_n\}$ is a sequence of Hilbert-Schmidt operators and thus compact. To show that the sequence converges to $g(\cdot)f(-i\boldsymbol{\nabla})$ in norm, we take $\psi \in L^2(\mathbb{R}^d)$ and see that

$$\left(f(-i\boldsymbol{\nabla}) - \phi_n f(-i\boldsymbol{\nabla})\right)\psi = \widecheck{f\hat{\psi}} - \widecheck{\phi_n f \hat{\psi}} \tag{3.41}$$

$$= \widecheck{f\hat{\psi} - \phi_n f \hat{\psi}} \tag{3.42}$$

$$= \widecheck{f[1-\phi_n]\hat{\psi}}, \tag{3.43}$$

due to the linearity of the Fourier transform. We note that for large n the function $[1-\phi_n(\boldsymbol{k})]$ is nonzero only for large $|\boldsymbol{k}|$. But then the assumption $\lim_{|\boldsymbol{k}|\to\infty} f(\boldsymbol{k}) = 0$ implies that $\forall \epsilon > 0, \exists N_\epsilon \in \mathbb{N}$ such that

$$\int |f(\boldsymbol{k})[1-\phi_n(\boldsymbol{k})]|^2 \, \mathrm{d}\boldsymbol{k} < \epsilon, \qquad \forall n \ge N_\epsilon. \tag{3.44}$$

Then by Plancherel's formula and (3.43), $\forall \epsilon > 0$ we can choose $N_\epsilon \in \mathbb{N}$ such that

$$\|g(\cdot)\left(f(-i\boldsymbol{\nabla}) - \phi_n f(-i\boldsymbol{\nabla})\right)\psi\|_{L^2}^2 < \epsilon \|g\|_{L^\infty}^2 \|\psi\|_{L^2}^2, \qquad n \ge N_\epsilon. \tag{3.45}$$

But as $g \in L^\infty(\mathbb{R}^d)$ we have that $\{T_n\}$ converges in norm to $g(\cdot)f(-i\boldsymbol{\nabla})$. □

Sometimes we will denote the operators $g(\cdot)f(-i\boldsymbol{\nabla})$ and $f(-i\boldsymbol{\nabla})$ as $g(\cdot)f(\boldsymbol{p})$ and $f(\boldsymbol{p})$ respectively. This is the case in the next lemma, which is needed to prove the HVZ theorem.

Lemma 3.3.2 *Let A be a self-adjoint operator with domain $D(A) \subseteq H^1(\mathbb{R}^d)$. If $\Omega \subset \mathbb{R}^d$ is a bounded subset, and χ_Ω the characteristic function of Ω given by*

$$\chi_\Omega(\boldsymbol{x}) := \begin{cases} 1, & \text{if } \boldsymbol{x} \in \Omega, \\ 0, & \text{if } \boldsymbol{x} \notin \Omega. \end{cases} \tag{3.46}$$

Then $\chi_\Omega(A-i)^{-1}$ is compact.

Proof. To prove the theorem we make use of the relation

$$\chi_\Omega(A-i)^{-1} = \chi_\Omega(1+|\boldsymbol{p}|^2)^{-\frac{1}{2}}(1+|\boldsymbol{p}|^2)^{\frac{1}{2}}(A-i)^{-1}. \tag{3.47}$$

The theorem can then be proven by showing that $(1+|\boldsymbol{p}|^2)^{\frac{1}{2}}(A-i)^{-1}$ is bounded on $L^2(\mathbb{R}^d)$, and that $\chi_\Omega(1+|\boldsymbol{p}|^2)^{-\frac{1}{2}}$ is compact, since the product of a bounded operator and a compact operator is compact. Let $\phi \in L^2(\mathbb{R}^d)$ then

$$\|(1+|\boldsymbol{p}|^2)^{\frac{1}{2}}(A-i)^{-1}\phi\|_{L^2} = \|(A-i)^{-1}\phi\|_{H^1}, \tag{3.48}$$

by the definition of the Sobolev spaces. The inverse of $A-i$ exists and is bounded, since $i \in \rho(A)$. It is defined on all of $L^2(\mathbb{R}^d)$, by the closed graph theorem, and maps to $D(A) \subset H^1(\mathbb{R}^d)$. This implies that

$$\|(1+|\boldsymbol{p}|^2)^{\frac{1}{2}}(A-i)^{-1}\phi\|_{L^2} < \infty, \tag{3.49}$$

for all $\phi \in L^2(\mathbb{R}^d)$. This shows boundedness. It remains to show that the operator $\chi_\Omega(1+|\boldsymbol{p}|^2)^{-\frac{1}{2}}$ is compact. But $\chi_\Omega \in L^2(\mathbb{R}^d)$ for a bounded $\Omega \subset \mathbb{R}^d$. Additionally, $(1+|\boldsymbol{p}|^2)^{-\frac{1}{2}}$ is bounded for all $\boldsymbol{p} \in \mathbb{R}^d$ and $\lim_{|\boldsymbol{p}|\to\infty}(1+|\boldsymbol{p}|^2)^{-\frac{1}{2}} = 0$, we can apply Lemma 3.3.1 to see that $\chi_\Omega(1+|\boldsymbol{p}|^2)^{-\frac{1}{2}}$ is compact. This concludes the proof. □

With this lemma proven, we are finally ready to prove the HVZ theorem. This is done in the next section.

3.4 HVZ Theorem

In Chapter 2 we associated an operator to the sesquilinear form of the system consisting of three interacting particles. As mentioned in the beginning of this chapter, we will determine the essential spectrum of that operator now. Recall that the operator is given by

$$H_{\lambda_1\lambda_2\lambda_3} = -\frac{1}{2}\frac{\partial^2}{\partial x^2} - \frac{1}{2}\frac{\partial^2}{\partial y^2} + \lambda_1\delta(x) + \lambda_2\delta(y) + \lambda_3\delta(x-y), \tag{3.50}$$

and we assumed that $\lambda_1, \lambda_2 < 0$ and $\lambda_3 > 0$.

The general idea behind the HVZ theorem is to consider subsystems, where at least one of the particles does not interact with the rest of the system. Then the energy of the subsystems is simply given by the kinetic energy of these specific particles, and the remaining system. As an example, the subsystem where one of the negatively charged particles does not interact with the rest of the system can be represented by the operator

$$H_{\lambda_1 00} = -\frac{1}{2}\frac{\partial^2}{\partial x^2} - \frac{1}{2}\frac{\partial^2}{\partial y^2} + \lambda_1 \delta(x), \tag{3.51}$$

where $\lambda_1 < 0$. Similar systems are represented by the operators $H_{0\lambda_2 0}$ and $H_{00\lambda_3}$. The HVZ theorem tells us that the infimum of the spectrums of these subsystems is the bottom of the essential spectrum of $H_{\lambda_1,\lambda_2,\lambda_3}$. Due to the assumption $\lambda_1, \lambda_2 < 0$ and $\lambda_3 \geq 0$, we know

$$\inf \sigma(H_{\lambda_1 00}), \inf \sigma(H_{0\lambda_2 0}) \leq \inf \sigma(H_{00\lambda_3}). \tag{3.52}$$

The operator $H_{\lambda_1 00}$ is the sum of the commuting self-adjoint operators

$$h_x := -\frac{1}{2}\frac{\partial^2}{\partial x^2} + \lambda_1 \delta(x), \quad \text{and} \quad h_y := -\frac{1}{2}\frac{\partial^2}{\partial y^2}. \tag{3.53}$$

By the results in Section XIII of [Reed and Simon, 1978] the spectrum of $H_{\lambda_1 00}$ is

$$\sigma(H_{\lambda_1 00}) = \sigma(h_x) + \sigma(h_y). \tag{3.54}$$

It is a standard result from physics, e.g. [Postma, 1984], that the operator h_x has a single discrete negative eigenvalue, which we denote $-E_{\lambda_1}$, given by

$$-E_{\lambda_1} = -\frac{\lambda_1^2}{2}. \tag{3.55}$$

By (3.54) and Theorem 3.1.3 we have that $\sigma(H_{\lambda_1 00}) = [-E_{\lambda_1}, \infty)$. Similar results hold for $H_{0\lambda_2 0}$ which has the spectrum $\sigma(H_{0\lambda_2 0}) = [-E_{\lambda_2}, \infty)$. We assume without loss of generality that $\lambda_1 \leq \lambda_2$, then $-E_{\lambda_1} \leq -E_{\lambda_2}$. We will show that $-E_{\lambda_1}$ is the bottom of the essential spectrum. For the more general case of a N-particle system we refer to [Cycon et al., 1987].

Theorem 3.4.1 (HVZ Theorem) *Let $H_{\lambda_1\lambda_2\lambda_3}$ be the operator given by* (3.50), *with $\lambda_1 \leq \lambda_2 < 0$ and $\lambda_3 \geq 0$. If $-E_1$ is infimum of the spectrum of $H_{\lambda_1 00}$, then*

$$\sigma_{ess}(H_{\lambda_1\lambda_2\lambda_3}) = [-E_{\lambda_1}, \infty). \tag{3.56}$$

Proof. The proof is split into two cases. First it is shown that $[-E_{\lambda_1}, \infty) \subseteq \sigma_{ess}(H_{\lambda_1\lambda_2\lambda_3})$, and afterwards that $\sigma_{ess}(H_{\lambda_1\lambda_2\lambda_3}) \subseteq [-E_{\lambda_1}, \infty)$. The first part is somewhat easier than the second part.

Let $E \in [-E_{\lambda_1}, \infty)$. Then a Weyl sequence for E and $H_{\lambda_1\lambda_2\lambda_3}$ is constructed, which shows that E is in the essential spectrum of $H_{\lambda_1\lambda_2\lambda_3}$. Since $-E_{\lambda_1}$ is an eigenvalue of $H_{\lambda_1 00}$ there exists $\phi_{\lambda_1} \in H^1(\mathbb{R})$, such that we can write

$$\left\{-\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}x^2} - \lambda_1\delta(x)\right\}\phi_{\lambda_1}(x) = -E_{\lambda_1}\phi_{\lambda_1}(x). \tag{3.57}$$

Define $\lambda := E + E_{\lambda_1} > 0$. Then $\lambda \in \sigma_{ess}(-\Delta)$ by Theorem 3.1.3. Weyl's criterion gives the existence of a Weyl sequence for $-\Delta$ on $H^2(\mathbb{R})$ and λ. Let $\{j_{n,\lambda}\}$ be such a Weyl sequence, the actual definition of $j_{n,\lambda}$ is contained in the proof of Theorem 3.1.3. By the definition of Weyl sequences

$$\left\|\left(-\frac{1}{2}\frac{\mathrm{d}^2}{\mathrm{d}y^2} - \lambda\right) j_{n,\lambda}(y)\right\| \to 0 \quad \text{for } n \to \infty. \tag{3.58}$$

Define the sequence $\{\Psi_n\} \subset H^1(\mathbb{R}^2)$ by

$$\Psi_n(x,y) := \phi_{\lambda_1}(x) j_{n,\lambda}(y). \tag{3.59}$$

We show that $\{\Psi_n\}$ is a Weyl sequence for $H_{\lambda_1\lambda_2\lambda_3}$ and E. The normalization of $\{\Psi_n\}$ follows from the fact that $j_{n,\lambda}$ and ϕ_{λ_1} are normalized. Let $\Phi \in L^2(\mathbb{R}^2)$, and consider

$$\langle \Phi, \Psi_n \rangle = \iint \overline{\Phi(x,y)}\Psi_n(x,y)\,\mathrm{d}x\,\mathrm{d}y \tag{3.60}$$

$$= \int j_{n,\lambda}(y) \int \overline{\Phi(x,y)}\phi_{\lambda_1}(x)\,\mathrm{d}x\,\mathrm{d}y. \tag{3.61}$$

The integral over x defines a function in y, and the weak convergence of of $\{j_{n,\lambda}\}$ implies that (3.61) goes to zero for $n \to \infty$. Thus $\{\Psi_n\}$ converges weakly to zero. It remains to show that

$$\|(H_{\lambda_1\lambda_2\lambda_3} - E)\,\Psi_n\| \to 0 \quad \text{for } n \to \infty. \tag{3.62}$$

The properties of the functions ϕ_{λ_1} and $j_{n,\lambda}$ gives that

$$\|(H_{\lambda_1\lambda_2\lambda_3} + E_{\lambda_1} - \lambda)\,\Psi_n\|^2 \le \left\{\|[\lambda_2\delta(y)\Psi_n\|^2 + \|\lambda_3\delta(x-y)\Psi_n\|^2\right\}, \tag{3.63}$$

with some abuse of notation. The right-hand side of (3.63) is to be understood as

$$\|[\lambda_2\delta(y)\Psi_n\|^2 + \|\lambda_3\delta(x-y)\Psi_n\|^2 = \lambda_2^2\int |\Psi_n(x,0)|^2\,\mathrm{d}x + \lambda_3^2\int |\Psi_n(x,x)|^2\,\mathrm{d}x. \tag{3.64}$$

The first term on the right-hand side of (3.64) is proportional to

$$\int |\Psi_n(x,0)|^2\,\mathrm{d}x = |j_{n,\lambda}(0)|^2\|\phi_{\lambda_1}\|^2, \tag{3.65}$$

which goes to zero for $n \to \infty$, since $\phi_{\lambda_1} \in L^2(\mathbb{R})$ and the definition of $j_{n,\lambda}$ in (3.4). Similarly, we see that the second term on the right-hand side of (3.64) is proportional to

$$\int_{\mathbb{R}} |\Psi_n(x,x)|^2 \, \mathrm{d}x = \frac{1}{n\|\varphi\|} \|\varphi_n \phi_{\lambda_1}\|^2, \tag{3.66}$$

which also goes to zero for $n \to \infty$. Thus (3.62) holds, and $\{\Psi_n\}$ is a Weyl sequence for E and $H_{\lambda_1\lambda_2\lambda_3}$. This concludes shows the first inclusion.

It remains to prove the inclusion $\sigma_{ess}(H_{\lambda_1\lambda_2\lambda_3}) \subseteq [-E_{\lambda_1}, \infty)$. To do this it is enough to show that $\sigma_{ess}(H_{\lambda_1\lambda_2\lambda_3}) \cap (-\infty, -E_{\lambda_1}) = \emptyset$. Let $f \in C_0^\infty(\mathbb{R})$ be a function with support in (a,b), where $b \leq -E_{\lambda_1}$. If $f(H_{\lambda_1\lambda_2\lambda_3})$ is a compact operator, it follows that there is only discrete eigenvalues of $H_{\lambda_1\lambda_2\lambda_3}$ in the interval (a,b). To show that $f(H_{\lambda_1\lambda_2\lambda_3})$ is compact, we want to construct a sequence of compact operators which converges to $f(H_{\lambda_1\lambda_2\lambda_3})$ in norm.

The Helffer-Sjöstrand formula, Theorem 3.2.1, gives

$$f(H_{\lambda_1\lambda_2\lambda_3}) = -\frac{1}{\pi} \int_{\Omega} \overline{\partial} \tilde{f_N}(z) (H_{\lambda_1\lambda_2\lambda_3} - z)^{-1} \, \mathrm{d}y \, \mathrm{d}x, \tag{3.67}$$

where $\tilde{f_N}(z)$ is the almost analytical extension of f with N terms, and $\Omega = [a,b] \times [-1,1]$. The idea is to construct a sequence of operators approximating the resolvent operator in Hellfer-Sjöstrands formula.

Let $\phi(x) \in C_0^\infty(\mathbb{R})$ be a function satisfying $0 \leq \phi(x) \leq 1$ and

$$\phi(x) = \begin{cases} 1, & \text{if } |x| \leq 1, \\ 0, & \text{if } |x| \geq 2. \end{cases} \tag{3.68}$$

We use ϕ to define a sequence of functions $\{\phi_n\}$ by $\phi_n(x) := \phi(x/n)$. Then

$$\phi_n(x) = \begin{cases} 1, & \text{if } |x| \leq n, \\ 0, & \text{if } |x| \geq 2n. \end{cases} \tag{3.69}$$

Note that the derivatives of $\phi_n(x)$ satisfy

$$\left| \frac{\mathrm{d}^\alpha}{\mathrm{d}x^\alpha} \phi_n(x) \right| \leq \frac{C_\alpha}{n^\alpha}, \tag{3.70}$$

where $\alpha \in \mathbb{N}_0$ and $C_\alpha > 0$. We then use ϕ_n to write

$$1 = (1 + \phi_n(x) - \phi_n(x))(1 + \phi_n(y) - \phi_n(y)) \tag{3.71}$$

$$= (1 - \phi_n(x))\phi_n(y) + (1 - \phi_n(y))\phi_n(x) + \phi_n(x)\phi_n(y) + (1 - \phi_n(x))(1 - \phi_n(y)). \tag{3.72}$$

Note that the term $(1-\phi_n(x))\phi_n(y)$ is only nonzero, when y is close to zero and x is away from zero, and similarly for the rest of the terms. This motivates a definition of the sequence of functions $\{S_n(z)\}$ given by

$$\begin{aligned} S_n(z) &:= (1-\phi_n(x))\phi_n(y)(H_{0\lambda_2\lambda_3}-z)^{-1} + (1-\phi_n(y))\phi_n(x)(H_{\lambda_1 0\lambda_3}-z)^{-1} \\ &\quad + \phi_n(x)\phi_n(y)(H_{\lambda_1\lambda_2\lambda_3}-z)^{-1} + (1-\phi_n(x))(1-\phi_n(y))(H_{00\lambda_3}-z)^{-1}. \end{aligned}$$

We want to use $S_n(z)$ to approximate $(H_{\lambda_1\lambda_2\lambda_3}-z)^{-1}$. To do this we need the following relation

$$(A-z)\varphi(A-z)^{-1} = [A,\varphi](A-z)^{-1} + \varphi(A-z)(A-z)^{-1}, \tag{3.73}$$

where $[\cdot,\cdot]$ is the commutator relation. Equation (3.73) and the fact that the terms of the type $\delta(x)(1-\phi_n(x))$ are zero, gives that

$$(H_{\lambda_1\lambda_2\lambda_3}-z)S_n(z) = \mathbb{I} + T_n(z), \tag{3.74}$$

where $T_n(z)$ is given by

$$\begin{aligned} T_n(z) &:= \left[H_{0\lambda_2\lambda_3}, (1-\phi_n(x))\phi_n(y)\right](H_{0\lambda_2\lambda_3}-z)^{-1} \\ &\quad + \left[H_{\lambda_1 0\lambda_3}, (1-\phi_n(y))\phi_n(x)\right](H_{\lambda_1 0\lambda_3}-z)^{-1} \\ &\quad + \left[H_{\lambda_1\lambda_2\lambda_3}, \phi_n(y)\phi_n(x)\right](H_{\lambda_1\lambda_2\lambda_3}-z)^{-1} \\ &\quad + \left[H_{00\lambda_3}, (1-\phi_n(x))(1-\phi_n(y))\right](H_{00\lambda_3}-z)^{-1}. \end{aligned} \tag{3.75}$$

If the resolvent exists, we write

$$S_n(z) = (H_{\lambda_1\lambda_2\lambda_3}-z)^{-1} + (H_{\lambda_1\lambda_2\lambda_3}-z)^{-1}T_n(z). \tag{3.76}$$

Isolating the resolvent operator in (3.76), we get

$$(H_{\lambda_1\lambda_2\lambda_3}-z)^{-1} = S_n(z) - (H_{\lambda_1\lambda_2\lambda_3}-z)^{-1}T_n(z). \tag{3.77}$$

This expression for the resolvent is inserted in Helffer-Sjöstrand's formula (3.67), to get

$$f(H_{\lambda_1\lambda_2\lambda_3}) = -\frac{1}{\pi}\int_\Omega \overline{\partial}\tilde{f}_N(z)\left[S_n(z) - (H_{\lambda_1\lambda_2\lambda_3}-z)^{-1}T_n(z)\right]\,\mathrm{d}y\,\mathrm{d}x. \tag{3.78}$$

Inserting the expression for $S_n(z)$ in (3.78) gives

$$\begin{aligned} f(H_{\lambda_1\lambda_2\lambda_3}) &= (1-\phi_n(x))\phi_n(y)f(H_{0\lambda_2\lambda_3}) + (1-\phi_n(y))\phi_n(x)f(H_{\lambda_1 0\lambda_3}) \\ &\quad + (1-\phi_n(x))(1-\phi_n(y))f(H_{00\lambda_3}) + \phi_n(x)\phi_n(y)f(H_{\lambda_1\lambda_2\lambda_3}) \\ &\quad + \frac{1}{\pi}\int_\Omega \overline{\partial}\tilde{f}_N(z)(H_{\lambda_1\lambda_2\lambda_3}-z)^{-1}T_n(z)\,\mathrm{d}y\,\mathrm{d}x. \end{aligned} \tag{3.79}$$

The terms with $f(H_{0\lambda_2\lambda_3})$, $f(H_{\lambda_1 0\lambda_3})$ and $f(H_{00\lambda_3})$ are zero. To see this consider Stone's formula, (A.18), and note that

$$\sigma(H_{\lambda_1 0\lambda_3}) \cap (a,b) = \emptyset, \quad \text{and } \sigma(H_{0\lambda_2\lambda_3}) \cap (a,b) = \emptyset, \tag{3.80}$$

since $\lambda_3 \geq 0$. The expression for $f(H_{\lambda_1\lambda_2\lambda_3})$ is then reduced to

$$f(H_{\lambda_1\lambda_2\lambda_3}) = \phi_n(x)\phi_n(y)f(H_{\lambda_1\lambda_2\lambda_3}) + \frac{1}{\pi}\int_{\Omega} \overline{\partial}\tilde{f_N}(z)R_{H_{\lambda_1\lambda_2\lambda_3}}(z)T_n(z)\,\mathrm{d}z, \quad (3.81)$$

where $R_{H_{\lambda_1\lambda_2\lambda_3}}(z) = (H_{\lambda_1\lambda_2\lambda_3} - z)^{-1}$. The first term in (3.81) is compact. To see this consider

$$\phi_n(x)\phi_n(y)f(H_{\lambda_1\lambda_2\lambda_3}) = \phi_n(x)\phi_n(y)(H+i)^{-1}(H+i)f(H_{\lambda_1\lambda_2\lambda_3}), \qquad (3.82)$$

but $\phi_n(x)\phi_n(y)(H+i)^{-1}$ is compact by Lemma 3.3.2, and $(H+i)f(H_{\lambda_1\lambda_2\lambda_3})$ is bounded, since f has compact support. The product of a compact and a bounded operator, is a compact operator. It remains to show that the last term in (3.82) goes to zero in norm for $n \to \infty$. Consider the commutator terms in $T_n(x)$ of the type

$$[H_{0\lambda_2\lambda_3}, (1-\phi_n(x))\phi_n(y)] = \phi_n(y)\left[-\frac{\mathrm{d}^2}{\mathrm{d}x^2}, \phi_n(x)\right] + (1-\phi_n(x))\left[-\frac{\mathrm{d}^2}{\mathrm{d}y^2}, \phi_n(y)\right]. \qquad (3.83)$$

Similar results hold for the other terms in $T_n(z)$. The commutators are calculated

$$\left[-\frac{\mathrm{d}^2}{\mathrm{d}x^2}, \phi_n(x)\right] = \left(-\phi_n''(x) - \phi_n'(x)\frac{\mathrm{d}}{\mathrm{d}x}\right), \qquad (3.84)$$

where primes denote the derivative with respect to x. Using (3.83), (3.84), (3.70) and (A.16) it follows that

$$\|(H_{\lambda_1\lambda_2\lambda_3} - z)^{-1}T_n(z)\Psi\| \leq \frac{C}{n|\operatorname{Im} z|^2}\|\Psi\|, \qquad (3.85)$$

where $C > 0$ and $\Psi \in L^2(\mathbb{R}^2)$. But $\overline{\partial}f_N(z)$ is proportional to $|\operatorname{Im} z|^N$ for small $\operatorname{Im} z$. If $N \geq 3$ the integral in (3.81) defines a bounded operator, with operator norm proportional to n^{-1}, which goes to zero for $n \to \infty$. Thus we have a sequence of compact operators which converge to $f(H_{\lambda_1\lambda_2\lambda_3})$ in norm. This implies that $f(H_{\lambda_1\lambda_2\lambda_3})$ is a compact operator, and have only discrete eigenvalues. This concludes the proof of the HVZ theorem. □

We have now proven the HVZ theorem, which gives the essential spectrum of the operator $H_{\lambda_1,\lambda_2,\lambda_3}$. We can use this information to determine the discrete eigenvalues, since they are in $\mathbb{R} \setminus \sigma_{ess}(H_{\lambda_1\lambda_2\lambda_3})$. In the next chapter, we prove a theorem which is central to determining the discrete eigenvalues of $H_{\lambda_1\lambda_2\lambda_3}$.

Chapter 4

The Resolvent Operator

In this chapter, we want to describe some results regarding the resolvent operator of the self-adjoint operator we constructed in chapter 2.

The resolvent operator of contains all information about the spectrum of the operator and is thus interesting to study when one wants to determine the spectrum. In the previous chapter, we determined the essential spectrum of the operator H given by (3.1). The discrete spectrum of H consist of the points $z \in \mathbb{R} \setminus \sigma_{ess}(H)$ where $H - z$ is singular.

We want to give a description of the resolvent operator of H using the resolvent of the free Hamiltonian. So we devote the next section to the resolvent of the free Hamiltonian.

4.1 Resolvent of the free Hamiltonian

In this section, we examine the resolvent of $-\Delta$ on $H^2(\mathbb{R}^2)$. We sometimes call $-\Delta$ for the free Hamiltonian, and the resolvent of $-\Delta$ for the free resolvent.

Let $\lambda \in \mathbb{C}$, where $\operatorname{Im} \lambda > 0$ and $\operatorname{Re} \lambda = 0$. By Theorem 3.1.3 we know that $\lambda^2 \in \rho(-\Delta)$, since $\lambda^2 < 0$. Then $(-\Delta - \lambda^2)^{-1}$ is a bounded linear operator on all of $L^2(\mathbb{R}^2)$. To see how $(-\Delta - \lambda^2)^{-1}$ acts on $\psi \in L^2(\mathbb{R}^2)$, note that

$$\begin{aligned} \left[(-\Delta - \lambda^2)^{-1}\psi\right](\boldsymbol{x}) &= \widecheck{(|\boldsymbol{k}|^2 - \lambda^2)^{-1}\hat{\psi}(\boldsymbol{k})}(\boldsymbol{x}) && (4.1) \\ &= \frac{1}{4\pi^2} \int \psi(\boldsymbol{y}) \int \frac{e^{i\boldsymbol{k}\cdot(\boldsymbol{x}-\boldsymbol{y})}}{|\boldsymbol{k}|^2 - \lambda^2} \, \mathrm{d}\boldsymbol{k} \, \mathrm{d}\boldsymbol{y}. && (4.2) \end{aligned}$$

The operator $(-\Delta - \lambda^2)$ is a case of the operator $f(i\boldsymbol{\nabla})$ which was defined in Section 3.3. We would like to determine the integral kernel of the free resolvent. We will denote the kernel by $R_0(\boldsymbol{x}, \boldsymbol{y}, \lambda^2)$. By Equation (4.2) the kernel is given by

$$R_0(\boldsymbol{x},\boldsymbol{y},\lambda^2) = \frac{1}{4\pi^2}\int \frac{e^{i\boldsymbol{k}\cdot(\boldsymbol{x}-\boldsymbol{y})}}{|\boldsymbol{k}|^2-\lambda^2}\,\mathrm{d}\boldsymbol{k}. \tag{4.3}$$

The integral in (4.3) does not have a nice closed form solution, but can be written using Bessel functions. From [Hislop and Sigal, 1996] or [Reed and Simon, 1975] we get the representation of the integral kernel of the free resolvent

$$R_0(\boldsymbol{x},\boldsymbol{y},\lambda^2) = \frac{i}{4}H_0^{(1)}(\lambda|\boldsymbol{x}-\boldsymbol{y}|), \tag{4.4}$$

where $H_0^{(1)}$ is the Bessel function of the third kind. The function $H_0^{(1)}$ is also called a Hankel function of first order. We will use the following upper bound for the resolvent kernel, which holds when $\operatorname{Im}\lambda > 0$ and $\boldsymbol{x} \neq \boldsymbol{y}$,

$$|R_0(\boldsymbol{x},\boldsymbol{y},\lambda^2)| \leq e^{-\operatorname{Im}\lambda|\boldsymbol{x}-\boldsymbol{y}|}(|\lambda||\boldsymbol{x}-\boldsymbol{y}|)^{-\frac{1}{2}}. \tag{4.5}$$

This bound follow from the properties of the Hankel function of first order, as described in [Galkowski and Smith, 2014] and [Abramowitz and Stegun, 1972], Chapter 9. In the next section we use this bound for the integral kernel to give an upper bound of the operator norm of the free resolvent. To do this we use Schur's test, which is stated in the following theorem.

Theorem 4.1.1 (Schur's Test) *Let $A : D(A) \to L^2(\mathbb{R}^n)$, where $D(A) \subset L^2(\mathbb{R}^n)$, be an integral operator with integral kernel $A(x,y)$. Then the operator norm of A is bounded by*

$$\|A\| \leq \max\left\{\sup_{\boldsymbol{y}\in\mathbb{R}^n}\int |A(\boldsymbol{x},\boldsymbol{y})|\,d\boldsymbol{y},\quad \sup_{\boldsymbol{x}\in\mathbb{R}^n}\int |A(\boldsymbol{x},\boldsymbol{y})|\,d\boldsymbol{x}\right\}. \tag{4.6}$$

Proof. Let $f \in D(A)$, and consider

$$|(Af)(\boldsymbol{x})| \leq \int |A(\boldsymbol{x},\boldsymbol{y})||f(\boldsymbol{y})|\,\mathrm{d}\boldsymbol{y} = \int |A(\boldsymbol{x},\boldsymbol{y})|^{\frac{1}{2}}|A(\boldsymbol{x},\boldsymbol{y})|^{\frac{1}{2}}|f(\boldsymbol{y})|\,\mathrm{d}\boldsymbol{y}. \tag{4.7}$$

Applying Cauchy-Schwarz's inequality we get that

$$|(Af)(\boldsymbol{x})| \leq \sqrt{\int |A(\boldsymbol{x},\boldsymbol{y})|\,\mathrm{d}\boldsymbol{y}}\sqrt{\int |A(\boldsymbol{x},\boldsymbol{y})||f(\boldsymbol{y})|^2\,\mathrm{d}\boldsymbol{y}}. \tag{4.8}$$

Squaring (4.8) we get that

$$|(Af)(\boldsymbol{x})|^2 \leq \left(\int |A(\boldsymbol{x},\boldsymbol{y})|\,\mathrm{d}\boldsymbol{y}\right)\left(\int |A(\boldsymbol{x},\boldsymbol{y})||f(\boldsymbol{y})|^2\,\mathrm{d}\boldsymbol{y}\right) \tag{4.9}$$

$$\leq C_1\int |A(\boldsymbol{x},\boldsymbol{y})||f(\boldsymbol{y})|^2\,\mathrm{d}\boldsymbol{y}, \tag{4.10}$$

where

$$C_1 := \sup_{\boldsymbol{x}\in\mathbb{R}^n}\int |A(\boldsymbol{x},\boldsymbol{y})|\,\mathrm{d}\boldsymbol{y}. \tag{4.11}$$

Using (4.10) and Fubini's Theorem we get that

$$\|Af\|_{L^2}^2 \leq C_1 \iint |A(\boldsymbol{x},\boldsymbol{y})| \,\mathrm{d}\boldsymbol{x} |f(\boldsymbol{y})|^2 \,\mathrm{d}\boldsymbol{y} \leq C_1 C_2 \|f\|_{L^2}^2, \tag{4.12}$$

where

$$C_2 := \sup_{\boldsymbol{y}\in\mathbb{R}^n} \int |A(\boldsymbol{x},\boldsymbol{y})| \,\mathrm{d}\boldsymbol{x}. \tag{4.13}$$

Choose $C := \max\{C_1, C_2\}$ and we see that

$$\|Af\|_{L^2} \leq C\|f\|_{L^2}, \tag{4.14}$$

this concludes the proof of Schur's test. □

This concludes the section on the free resolvent. We use the bound for the integral kernel and Schur's test in the next section.

4.2 Resolvent of the Operator

In this section, we examine the resolvent of H, where H is the operator associated to the sesquilinear form Q given by (2.42). The section concludes with a result which can be used to determine the discrete eigenvalues of H.

By Theorem 2.1.1 there exists a bounded trace operator $\tau : H^1(\mathbb{R}^2) \to L^2(\mathbb{R})$. Let $\psi \in H^1(\mathbb{R}^2)$, then we define the operators τ_1, τ_2 and τ_3 by

$$[\tau_1\psi](x,y) := \psi(x,0) \tag{4.15}$$

$$[\tau_2\psi](x,y) := \psi(0,y) \tag{4.16}$$

$$[\tau_3\psi](x,y) := \psi(x,x). \tag{4.17}$$

Then we can define an operator $\tau : H^1(\mathbb{R}^2) \to \bigoplus_{i=1}^3 L^2(\mathbb{R})$ as $\tau := (\tau_1, \tau_2, \tau_3)$. Using τ we write the operator H as

$$H = H_0 + \tau^* g \tau, \tag{4.18}$$

where $H_0 = -\frac{1}{2}\frac{\partial^2}{\partial x^2} - \frac{1}{2}\frac{\partial^2}{\partial x^2}$, and g is the 3×3 matrix defined by

$$g := \begin{bmatrix} \lambda_1 & 0 & 0 \\ 0 & \lambda_2 & 0 \\ 0 & 0 & \lambda_3 \end{bmatrix}. \tag{4.19}$$

We want to use the expression in (4.18) to express the resolvent of H. Let $\lambda \in \mathbb{C}$ with $\operatorname{Im}\lambda > 0$ and $\operatorname{Re}\lambda = 0$. Define $-M := \lambda^2 < 0$, and let us write $H + M$ as

$$H + M = (H_0 + M)^{\frac{1}{2}}(\mathbb{1} + (H_0 + M)^{-\frac{1}{2}}\tau^* g \tau (H_0 + M)^{-\frac{1}{2}})(H_0 + M)^{\frac{1}{2}}. \tag{4.20}$$

We will use this expression to express the resolvent. To do this we need the next lemma.

Lemma 4.2.1 *Let H_0 be the free Hamiltonian and $-M = \lambda^2$, where $\lambda \in \mathbb{C}$ with* $\operatorname{Im}\lambda > 0$ *and* $\operatorname{Re}\lambda = 0$*. Then the operator*

$$(H_0 + M)^{-\frac{1}{2}}\tau^* g \tau (H_0 + M)^{-\frac{1}{2}} \tag{4.21}$$

in (4.20) *is bounded on $L^2(\mathbb{R}^2)$.*

Proof. Ignoring the constants $\lambda_\alpha \in \mathbb{R}$, the operator in (4.21) consists of three terms of the type

$$(H_0 + M)^{-\frac{1}{2}}\tau_\alpha^* \tau_\alpha (H_0 + M)^{-\frac{1}{2}}, \tag{4.22}$$

where $\alpha \in \{1, 2, 3\}$. We show that each term is bounded. Let $\Phi, \Psi \in L^2(\mathbb{R}^2)$, then the operator in (4.22) is defined by the sesquilinear form

$$\langle \Phi, (H_0+M)^{-\frac{1}{2}}\tau_\alpha^* \tau_\alpha (H_0+M)^{-\frac{1}{2}}\Psi\rangle = \langle \tau_\alpha (H_0+M)^{-\frac{1}{2}}\Phi, \tau_\alpha (H_0+M)^{-\frac{1}{2}}\Psi\rangle. \tag{4.23}$$

To see that this is bounded on $L^2(\mathbb{R}^2)$, note that $(H_0 + M)^{-\frac{1}{2}}\Psi \in H^1(\mathbb{R}^2)$ for all $\Psi \in L^2(\mathbb{R}^2)$, since $D(H_0) \subset H^1(\mathbb{R}^2)$. The operator τ_α is defined on $H^1(\mathbb{R}^2)$ and bounded by Theorem 2.1.1. This implies that the sesquilinear form in (4.23) is bounded. Riesz representation gives that the operator in (4.22) is bounded. Similar considerations hold for the remaining terms in (4.21). □

We want to expand the operator

$$\mathbb{1} + (H_0 + M)^{-\frac{1}{2}}\tau^* g \tau (H_0 + M)^{-\frac{1}{2}} \tag{4.24}$$

in a Neumann series. The next result guarantees that we can always choose M sufficiently large to do that.

Theorem 4.2.2 *There exists $\lambda \in C$, with* $\operatorname{Im}\lambda > 0$ *and* $\operatorname{Re}\lambda = 0$*, such that*

$$\|(H_0 + M)^{-\frac{1}{2}}\tau^* g \tau (H_0 + M)^{-\frac{1}{2}}\| < 1, \tag{4.25}$$

where $-M = \lambda^2$.

Proof. By Lemma 4.2.1 the operator in (4.25) is bounded. Then Riesz representation guarantees

$$\|(H_0 + M)^{-\frac{1}{2}}\tau_\alpha^* \tau_\alpha (H_0 + M)^{-\frac{1}{2}}\| = \sup_{\substack{\|\Phi\|=1 \\ \|\Psi\|=1}} |\langle \tau_\alpha (H_0 + M)^{-\frac{1}{2}}\Phi, \tau_\alpha (H_0 + M)^{-\frac{1}{2}}\Psi\rangle|,$$

for $\alpha \in \{1, 2, 3\}$. Using the Cauchy-Schwarz inequality on the right-hand side we see that

$$\|(H_0 + M)^{-\frac{1}{2}}\tau_\alpha^* \tau_\alpha (H_0 + M)^{-\frac{1}{2}}\| \le \|\tau_\alpha (H_0 + M)^{-\frac{1}{2}}\|^2. \tag{4.26}$$

We let $\Psi \in L^2(\mathbb{R}^2)$, and use that τ is bounded and Plancherel's theorem to find

$$\|\tau_\alpha(H_0+M)^{-\frac{1}{2}}\Psi\|^2 \leq C\|(H_0+M)^{-\frac{1}{2}}\Psi\|^2 = C\|(|\boldsymbol{k}|^2+M)^{-\frac{1}{2}}\hat{\Psi}\|^2, \qquad (4.27)$$

for some constant $C > 0$. We can then write

$$\|\tau_\alpha(H_0+M)^{-\frac{1}{2}}\Psi\|^2 \leq C\int_{\mathbb{R}^2} \frac{|\hat{\Psi}(\boldsymbol{k})|^2}{|\boldsymbol{k}|^2+M}\,\mathrm{d}\boldsymbol{k}. \qquad (4.28)$$

But $M > 0$, so $(|\boldsymbol{k}|^2+M)^{-1} \leq M^{-1}$ for all $\boldsymbol{k} \in \mathbb{R}^2$. Finally we find that

$$\|\tau_\alpha(H_0+M)^{-\frac{1}{2}}\|^2 \leq \frac{C}{M}. \qquad (4.29)$$

Then (4.29) combined with (4.26) shows that we can always choose M such that (4.25) holds. □

If the inverse of (4.20) exists, we see that the following identity must hold.

$$(H+M)^{-1} = (H_0+M)^{-\frac{1}{2}}(\mathbb{1}+(H_0+M)^{-\frac{1}{2}}\tau^*g\tau(H_0+M)^{-\frac{1}{2}})^{-1}(H_0+M)^{-\frac{1}{2}}. \quad (4.30)$$

By Theorem 4.2.2 and Theorem A.1.6 we can choose $M > 0$ such that we can expand the operator in (4.24) in a Neumanns series given by

$$(\mathbb{1}+(H_0+M)^{-\frac{1}{2}}\tau^*g\tau(H_0+M)^{-\frac{1}{2}})^{-1} = \sum_{j=0}^{\infty}(-1)^j\left[(H_0+M)^{-\frac{1}{2}}\tau^*g\tau(H_0+M)^{-\frac{1}{2}}\right]^j.$$

Inserting this in (4.30) we find that

$$\begin{aligned}(H+M)^{-1} &= (H_0+M)^{-\frac{1}{2}} \\ &\quad\times\sum_{j=0}^{\infty}(-1)^j\left[(H_0+M)^{-\frac{1}{2}}\tau^*g\tau(H_0+M)^{-\frac{1}{2}}\right]^j(H_0+M)^{-\frac{1}{2}}.\end{aligned} \qquad (4.31)$$

Writing the terms of the sum, we get that

$$\begin{aligned}(H+M)^{-1} &= (H_0+M)^{-1} - (H_0+M)^{-1}\tau^*g\tau(H_0+M)^{-1} \\ &\quad + (H_0+M)^{-1}\tau^*g\tau(H_0+M)^{-1}\tau^*g\tau(H_0+M)^{-1} - \cdots .\end{aligned} \qquad (4.32)$$

We want to use the Neumann expansion to rearrange the terms again. To do this we need the next result.

Theorem 4.2.3 *There exists $M > 0$ such that*

$$\|\tau(H_0+M)^{-1}\tau^*g\| < 1, \qquad (4.33)$$

where H_0 is the free resolvent and g is given by (4.19).

Proof. Let us define $-M := \lambda^2$, where $\operatorname{Im}\lambda > 0$ and $\operatorname{Re}\lambda = 0$. The operator $\tau(H_0 + M)^{-1}\tau^* g$ is a 3×3 matrix consisting of elements of the type

$$\lambda_\beta \tau_\alpha (H_0 + M)^{-1} \tau_\beta^*, \tag{4.34}$$

where $\alpha, \beta \in \{1, 2, 3\}$. But the operator τ_α is simply a restriction to a line in $\mathbb{R}^2$. By (4.4), we have that the operator $\tau_\alpha(H_0 + M)^{-1}\tau_\beta^*$ must have the integral kernel

$$R_0(\boldsymbol{x}_\alpha, \boldsymbol{y}_\beta, \lambda^2) = \frac{i}{4} H_0^{(1)}(\lambda |\boldsymbol{x}_\alpha - \boldsymbol{y}_\beta|), \tag{4.35}$$

where $\boldsymbol{x}_\alpha$ and $\boldsymbol{y}_\beta$ are points on the lines corresponding to the operators τ_α and τ_β respectively. If we apply Schur's test, Theorem 4.1.1, we see that

$$\|\tau_\alpha (H_0 + M)^{-1} \tau_\beta^*\| \le \sup_{\boldsymbol{x}_\alpha} \frac{1}{4} \int_\beta |H_0^{(1)}(\lambda |\boldsymbol{x}_\alpha - \boldsymbol{y}_\beta|)| \, \mathrm{d}\boldsymbol{y}_\beta \tag{4.36}$$

$$= \frac{1}{4} \int_\beta |H_0^{(1)}(\lambda |\boldsymbol{y}_\beta|)| \, \mathrm{d}\boldsymbol{y}_\beta, \tag{4.37}$$

where we integrate over the line corresponding to τ_β. If we use the upper bound from (4.5) we can write

$$\|\tau_\alpha (H_0 + M)^{-1} \tau_\beta^*\| \le \int_0^\infty e^{-|\lambda| y} (|\lambda| y)^{-\frac{1}{2}} \, \mathrm{d}y = \frac{\sqrt{\pi}}{|\lambda|}. \tag{4.38}$$

This shows that we can always choose λ and thus M large enough such that (4.33) holds. □

By Theorem 4.2.3, we can choose $M > 0$ such that the following identity holds

$$g \sum_{j=0}^\infty (-1)^j \left[\tau (H_0 + M)^{-1} \tau^* g\right]^j = (g^{-1} + \tau (H_0 + M)^{-1} \tau^*)^{-1}. \tag{4.39}$$

Inserting this in (4.32) we find

$$(H + M)^{-1} = (H_0 + M)^{-1} - (H_0 + M)^{-1} [g^{-1} + \tau (H_0 + M)^{-1} \tau^*]^{-1} (H_0 + M)^{-1}. \tag{4.40}$$

Using analytic continuation we see that $(H - z)^{-1}$ exists for all $z \in \mathbb{C}$ where

$$[g^{-1} + \tau (H_0 - z)^{-1} \tau^*]^{-1} \tag{4.41}$$

exists. Writing $R_0(z)$ for the free resolvent and $R(z)$ for the resolvent of H we finally get that

$$R(z) = R_0(z) - R_0(z) [g^{-1} + \tau R_0(z) \tau^*]^{-1} R_0(z). \tag{4.42}$$

The final result of this chapter follows from the Theorem 3.4.1, the HVZ theorem, and the identity in (4.42). The result gives a condition for identifying points in the discrete spectrum of H.

Theorem 4.2.4 *Let H be the operator given by* (4.18)*, and let* $-E_{\lambda_1} = \inf \sigma_{ess}(H)$. *Then $E < -E_{\lambda_1}$ is a discrete eigenvalue of H if and only if*

$$\ker(g^{-1} + \tau R_0(E)\tau^*) \neq \{0\}. \tag{4.43}$$

Theorem 4.2.4 is the foundation for determining the existence of discrete eigenvalues of the system with Dirac delta interactions. We will not determine the existence of any actual eigenvalues in this project, but instead, consider another case of the three-body quantum system in one-dimension. The actual work of determining the eigenvalues of the system with Dirac delta interactions is carried out in the article [Cornean et al., 2006] and is done using a string of symmetry arguments. It was also done numerically in the article [Rosenthal, 1971].

Chapter 5

Perturbation Theory and the Feshbach Formula

In this chapter, we study another case of the three-body system in one-dimension. The system is formally described by the Schrödinger operator

$$H_\kappa = -\frac{1}{2}\frac{\partial^2}{\partial x^2} - \frac{1}{2}\frac{\partial^2}{\partial y^2} - v(x-y) + \kappa v(x) - \kappa v(y), \tag{5.1}$$

where $v \in C_0^\infty(\mathbb{R})$. Furthermore we assume that v is even, non-negative and satisfies

$$\int_{-\infty}^{\infty} v(x)\,\mathrm{d}x = 1. \tag{5.2}$$

This is a bit different from the system considered in the previous chapters, where the interaction v was a Dirac delta distribution. Similarly to what was done in Chapter 2, we could define H_κ from a sesquilinear form, show that it was a self-adjoint operator and give a specific description of the domain. We will skip the mathematical rigors and simply state that the domain of H_κ is $H^2(\mathbb{R}^2)$.

The physical interpretation of the system is that it consists of a nucleus with infinite mass and positive charge, and two particles with mass one. The two particles with finite mass have opposite charges. Since the nucleus has infinite mass there is no kinetic energy associated with the nucleus. The two particles with finite mass interact with the nucleus, the strength of the interaction is controlled by the coupling constant κ. This system can be used as a model for excitons in a one-dimensional semi-conductor. An exciton is the bound state of a hole and an electron.

We can write the Schrödinger operator of the system as

$$H_\kappa = H_0 - \kappa V. \tag{5.3}$$

We assume that the spectrum of H_0 is known and that κV is a small perturbation, specifically that $0 \leq \kappa \ll 1$. We want to apply perturbation theory to determine the spectrum of H_κ from the spectrum of H_0. Specifically, we want to use the Feshbach formula to study the eigenvalues of H_κ.

5.1 The Feshbach Formula

In this section, we will briefly introduce the Feshbach formula. For more information on and proofs of the Feshbach formula we refer to [Howland, 1975] and [Cornean, 2008].

We consider a self-adjoint operator H, with domain $D(H) \subset \mathcal{H}$, where $\mathcal{H}$ is a Hilbert space. We assume that H can be written as

$$H = H_0 - V, \tag{5.4}$$

where H_0 is the operator of a solvable model, and V is a perturbation. If Π_{eff} is an orthogonal projection, we define $\Pi_\perp := \mathbf{1} - \Pi_{\text{eff}}$. Then the decomposition of $\mathcal{H}$ in $\mathcal{H}_{\text{eff}} \oplus \mathcal{H}_\perp$ is allowed.

Let us denote by $H_{\text{eff}} := \Pi_{\text{eff}} H \Pi_{\text{eff}}$, $V_{\text{eff},\perp} := \Pi_{\text{eff}} V \Pi_\perp$ and $H_\perp := \Pi_\perp H \Pi_\perp$. If Π_{eff} commutes with H, we can write H as the following 2×2 matrix

$$H = \begin{bmatrix} H_{\text{eff}} & -V_{\text{eff},\perp} \\ -V_{\perp,\text{eff}} & H_\perp \end{bmatrix}. \tag{5.5}$$

The Feshbach formula gives that if the resolvent exists for $z \in \mathbb{C}$, then it can be written as the 2×2 matrix of operators

$$(H - z)^{-1} = \begin{bmatrix} S_W & -S_W V R \\ -R V S_W & R + R V S_W V R \end{bmatrix}, \tag{5.6}$$

where

$$R(z) := [\Pi_\perp (H - z) \Pi_\perp]^{-1} \tag{5.7}$$

$$W(z) := -\Pi_{\text{eff}} V R(z) V \Pi_{\text{eff}} \tag{5.8}$$

$$S_W(z) := (H_{\text{eff}} + W(z) - z)^{-1}. \tag{5.9}$$

Consequently the eigenvalues of H is exactly the points where either $R(z)$ or $S_W(z)$ is singular.

5.2 Application of the Feshbach Formula to H_κ

In this section, we want to use Feshbach's formula on the operator H_κ given by (5.1), with domain $H^2(\mathbb{R}^2)$. Before we do that, we have some general considerations regarding the operator H_κ.

It can be shown that the HVZ theorem holds for H_κ. Recall from Section 3.4 that the HVZ theorem relates the essential spectrum of a system with infimum of the spectrum of subsystems, where at least one particle does not interact with the rest of the system. The possible subsystems can be represented by the operators:

$$\begin{aligned} H_0 &= -\frac{1}{2}\frac{\partial^2}{\partial x^2} - \frac{1}{2}\frac{\partial^2}{\partial y^2} - v(x-y) \\ H_1 &= -\frac{1}{2}\frac{\partial^2}{\partial x^2} - \frac{1}{2}\frac{\partial^2}{\partial y^2} - \kappa v(y) \\ H_2 &= -\frac{1}{2}\frac{\partial^2}{\partial x^2} - \frac{1}{2}\frac{\partial^2}{\partial y^2} + \kappa v(x) \end{aligned}$$

If κ is small enough, then $\sigma_{ess}(H_\kappa) = [\min \sigma(H_0), \infty)$ where $\min \sigma(H_0) < 0$.

We perform a change of coordinates to a center of mass frame, where the coordinates are given by $s = x - y$ and $t = \frac{1}{2}(x+y)$. The operator in (5.1) is unitarily equivalent to the operator

$$H_\kappa = -\frac{1}{4}\frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial s^2} - v(s) + \kappa v\left(t + \frac{1}{2}s\right) - \kappa v\left(t - \frac{1}{2}s\right). \tag{5.10}$$

Write $H_\kappa = H_0 - \kappa V$, where

$$H_0 = -\frac{1}{4}\frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial s^2} - v(s), \qquad V = v\left(t - \frac{1}{2}s\right) - v\left(t + \frac{1}{2}s\right). \tag{5.11}$$

The operator H_0 is the sum of two operators with distinct variables. Then we can write H_0 as an operator on $L^2(\mathbb{R}) \otimes L^2(\mathbb{R})$, where $\otimes$ denotes the tensor product. We get

$$H_0 = h_t \otimes \mathbb{1} + \mathbb{1} \otimes h_s, \tag{5.12}$$

where $h_t = -\frac{1}{4}\frac{\partial^2}{\partial t^2}$ and $h_s = -\frac{\partial^2}{\partial s^2} - v(s)$. It can be shown that both h_t and h_s are self-adjoint operators. By Theorem 3.1.3 we know that $\sigma(h_t) = [0, \infty)$. Assume that h_s have a negative non-degenerate discrete eigenvalue denoted by $-E_0$, with corresponding eigenstate $\Psi \in H^2(\mathbb{R})$. The eigenstate Ψ is even, have exponential decay and can be chosen to be strictly positive and normalized. By results in Section XIII.9 of [Reed and Simon, 1978], we know that

$$\sigma(\mathbb{1} \otimes h_s) = \sigma(h_s), \qquad \text{and} \qquad \sigma(h_t \otimes \mathbb{1}) = \sigma(h_t), \tag{5.13}$$

and

$$\sigma(H_0) = \sigma(h_s) + \sigma(h_t). \tag{5.14}$$

Consequently, the spectrum of H_0 must be $\sigma(H_0) = [-E_0, \infty)$ and by the previous discussion about the essential spectrum we know that $\sigma_{ess}(H_\kappa) = [-E_0, \infty)$.

To apply the Feshbach formula we need an orthogonal projection, which maps the domain of H_κ to itself. Let us define the rank 1 projector on $L^2(\mathbb{R})$ by

$$P := |\Psi\rangle\langle\Psi|, \tag{5.15}$$

using Dirac bracket notation. Similarly we define the projector $\Pi := \mathbb{1} \otimes P$ on $L^2(\mathbb{R}) \otimes L^2(\mathbb{R})$. Let $\Phi \in L^2(\mathbb{R}^2)$, then Π acts on Φ by

$$[\Pi\Phi](s,t) = \Psi(s) \int \overline{\Psi(s')}\Phi(s',t)\,\mathrm{d}s'. \tag{5.16}$$

We prove that Π maps the domain of H_κ to itself, that Π is an orthogonal projection and that Π commutes with H_0.

Theorem 5.2.1 *The projector* $\Pi = \mathbb{1} \otimes P$ *maps* $H^2(\mathbb{R}^2)$ *to* $H^2(\mathbb{R}^2)$.

Proof. Let $\Phi \in H^2(\mathbb{R}^2)$. By the definition of Sobolev spaces in Definition A.3.2 and Plancherel's theorem, it is enough to show that $\Pi\Phi \in L^2(\mathbb{R}^2)$ and $\Delta(\Pi\Phi) \in L^2(\mathbb{R}^2)$. Applying Fubini's theorem and the Cauchy-Schwarz inequality we get

$$\begin{aligned}
\|\Pi\Phi\|_{L^2}^2 &= \iint \left|\Psi(s) \int \overline{\Psi(s')}\Phi(s',t)\,\mathrm{d}s'\right|^2 \mathrm{d}s\,\mathrm{d}t && (5.17)\\
&\le \iint |\Psi(s)|^2 \left|\int \overline{\Psi(s')}\Phi(s',t)\,\mathrm{d}s'\right|^2 \mathrm{d}s\,\mathrm{d}t && (5.18)\\
&\le \int \left(\int |\Psi(s')|^2\,\mathrm{d}s'\right)\left(\int |\Phi(s',t)|^2\,\mathrm{d}s'\right)\mathrm{d}t && (5.19)\\
&= \|\Phi\|_{L^2}^2 < \infty. && (5.20)
\end{aligned}$$

Since $\Phi \in H^2(\mathbb{R}^2) \subset L^2(\mathbb{R}^2)$. Similarly we show that $\Delta(\Pi\Phi) \in L^2(\mathbb{R}^2)$,

$$\begin{aligned}
\|\Delta(\Pi\Phi)\|_{L^2}^2 &= \iint \left|\left(\frac{\partial^2}{\partial t^2} + \frac{\partial^2}{\partial s^2}\right)\Psi(s)\int \overline{\Psi(s')}\Phi(s',t)\,\mathrm{d}s'\right|^2 \mathrm{d}s\,\mathrm{d}t && (5.21)\\
&\le \left\|\Psi''\right\|_{L^2}^2 \|\Phi\|_{L^2}^2 + \left\|\frac{\partial^2}{\partial t^2}\Phi(s,t)\right\|_{L^2}^2 < \infty. && (5.22)
\end{aligned}$$

It is finite, since $\Phi \in H^2(\mathbb{R}^2)$ and $\Psi \in H^2(\mathbb{R})$. Thus Π maps $H^2(\mathbb{R}^2)$ to $H^2(\mathbb{R}^2)$.□

Theorem 5.2.2 *The operator* $\Pi = \mathbb{1} \otimes P$ *is an orthogonal projection* $L^2(\mathbb{R}^2)$.

Proof. We begin by showing that $\Pi^2 = \Pi$. Let $\Phi \in L^2(\mathbb{R}^2)$, then

$$\begin{aligned}
[\Pi^2\Phi](s,t) &= \Psi(s)\int \overline{\Psi(s'')}\Psi(s'') \int \overline{\Psi(s')}\Phi(s',t)\,\mathrm{d}s'\,\mathrm{d}s'' && (5.23)\\
&= \Psi(s)\int \Psi(s'')|^2\,\mathrm{d}s'' \int \overline{\Psi(s')}\Phi(s',t)\,\mathrm{d}s' = [\Pi\Psi](s,t), && (5.24)
\end{aligned}$$

since Ψ is normalized. It remains to show that Π is self-adjoint. Consider the product

$$\begin{aligned}
\langle\Phi, \Pi\Phi\rangle &= \iint \overline{\Phi(s,t)}\Psi(s)\int \overline{\Psi(s')}\Phi(s',t)\,\mathrm{d}s'\,\mathrm{d}s\,\mathrm{d}t && (5.25)\\
&= \int \left(\int \overline{\Phi(s,t)}\Psi(s)\,\mathrm{d}s\right)\left(\int \overline{\Psi(s')}\Phi(s',t)\,\mathrm{d}s'\right)\mathrm{d}t = \langle\Pi\Phi, \Phi\rangle, && (5.26)
\end{aligned}$$

and we see that Π is self-adjoint, and thus an orthogonal projection. □

Theorem 5.2.3 *The operator* Π *commutes with* H_0.

Proof. Let $\Phi \in D(H_0) = H^2(\mathbb{R}^2)$. By Theorem 5.2.1 we have that Π maps $D(H_0)$ to $D(H_0)$, and thus $H_0\Pi$ is an operator on $D(H_0)$. Consider

$$[\Pi H_0 \Phi](s,t) = \Psi(s) \int \overline{\Psi(s')} \left(-\frac{1}{4}\frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial s'^2} - v(s') \right) \Phi(s',t)\,\mathrm{d}s'. \tag{5.27}$$

We can write

$$\Psi(s) \int \overline{\Psi(s')} \left(-\frac{1}{4}\frac{\partial^2}{\partial t^2} \right) \Phi(s',t)\,\mathrm{d}s' = -\frac{1}{4}\frac{\partial^2}{\partial t^2}\Psi(s) \int \overline{\Psi(s')}\Phi(s',t)\,\mathrm{d}s'. \tag{5.28}$$

Similarly, because $h_s = -\frac{\partial^2}{\partial s^2} - v(s)$ is self-adjoint and Ψ is an eigenstate of h_s belonging to the eigenvalue $-E_0$ we get

$$\Psi(s) \int \overline{\Psi(s')} \left(-\frac{\partial^2}{\partial s'^2} - v(s') \right) \Phi(s',t)\,\mathrm{d}s' = -E_0\Psi(s) \int \overline{\Psi(s')}\Phi(s',t)\,\mathrm{d}s'. \tag{5.29}$$

From (5.27), (5.28) and (5.29) we conclude that

$$[\Pi H_0 \Phi](s,t) = \left(-\frac{1}{4}\frac{\partial^2}{\partial t^2} - E_0 \right) \Psi(s) \int \overline{\Psi(s')}\Phi(s',t)\,\mathrm{d}s' = [H_0 \Pi \Phi](s,t), \tag{5.30}$$

and thus Π and H_0 commutes. □

We would like to use the Feshbach formula, in Equation (5.5), to determine eigenvalues of H_κ near $-E_0$. We let the operator Π correspond to Π_{eff} in the Feshbach formula, and define the operator $\Pi_\perp := \mathbb{1} \otimes P_\perp$. It can be shown that $\Pi_\perp$ is also an orthogonal projection and commutes with H_0. First we determine an interval around $-E_0$ where $R(z) = [\Pi_\perp(H_\kappa - z)\Pi_\perp]^{-1}$ exists. For that we need the following lemma.

Lemma 5.2.4 *Let* $-E_0 = \min \sigma(h_s)$. *Then there exists* $z_0 > 0$ *such that*

$$[\Pi_\perp(H_0 - z)\Pi_\perp]^{-1}, \tag{5.31}$$

exists and is bounded for $|z + E_0| < z_0$.

Proof. We show that there exists a $z_0 > 0$, for which $|z + E_0| < z_0$ implies that $\Pi_\perp(H_0 - z)\Pi_\perp > 0$. Recall that we write $H_0 = h_t \otimes \mathbb{1} + \mathbb{1} \otimes h_s$. Let $\Phi \in D(H_0)$ and consider the product

$$\langle \Phi, \Pi_\perp(h_t \otimes \mathbb{1})\Pi_\perp \Phi \rangle = \langle \Pi_\perp \Phi, (h_t \otimes \mathbb{1})\Pi_\perp \Phi \rangle \geq 0. \tag{5.32}$$

The first equality follows since $\Pi_\perp$ is an orthogonal projection. The inequality holds because $h_t \otimes \mathbb{1}$ is a positive operator. Similarly, we get that

$$\langle \Phi, \Pi_\perp(\mathbb{1} \otimes h_s)\Pi_\perp \Phi \rangle = \langle \Pi_\perp \Phi, (\mathbb{1} \otimes h_s)\Pi_\perp \Phi \rangle. \tag{5.33}$$

Since $\mathbb{1} \otimes h_s$ is a self-adjoint operator, we can use the spectral theorem to write

$$\langle \Phi, [\mathbb{1} \otimes (h_s - z)]\Phi\rangle = \int_{\sigma(h_s)} (\lambda - z)\, \mathrm{d}\mu_\Phi(\lambda). \tag{5.34}$$

Similarly, we get that

$$\langle \Pi_\perp \Phi, \mathbb{1} \otimes [(h_s - z)]\Pi_\perp \Phi\rangle = \int_{\sigma(h_s)} (\lambda - z)\, \mathrm{d}\mu_{\Pi_\perp \Phi}(\lambda) \tag{5.35}$$

$$= \int_{\sigma(h_s)\setminus\{-E_0\}} (\lambda - z)\, \mathrm{d}\mu_\Phi(\lambda), \tag{5.36}$$

since $\Pi_\perp$ is a projection on the orthogonal complement of the eigenspace belonging to $-E_0$. Define $E_1 := \min\{\sigma(h_s) \setminus \{-E_0\}\}$, and note that $E_1 \leq 0$, then

$$\langle \Pi_\perp \Phi, [\mathbb{1} \otimes (h_s - z)]\Pi_\perp \Phi\rangle \geq (E_1 - z) \int_{\sigma(h_s)\setminus\{-E_0\}} 1\, \mathrm{d}\mu_\Phi(\lambda) = (E_1 - z)\|\Pi_\perp \Phi\| > 0, \tag{5.37}$$

for z satisfying $|z + E_0| < \frac{|E_1+E_0|}{2}$. Thus $\Pi_\perp(H_0 - z)\Pi_\perp$ is invertible for all such z.

We now show that the inverse is bounded aswell. Let $\sigma(\Pi_\perp H_0 \Pi_\perp) := \sigma(h_t) + \sigma(h_s)\setminus\{-E_0\}$, and note that $E_1 \leq \min \sigma(\Pi_\perp H_0 \Pi_\perp)$. Then by the spectral theorem we can write

$$\langle \Phi, \Pi_\perp(H_0 - z)\Pi_\perp \Phi\rangle = \int_{\sigma(\Pi_\perp H_0 \Pi_\perp)} (\lambda - z)\, \mathrm{d}\mu_\Phi(\lambda). \tag{5.38}$$

The norm of the inverse can be calculated by

$$\|(\Pi_\perp(H_0 - z)\Pi_\perp)^{-1}\Phi\|^2 = \langle (\Pi_\perp(H_0 - z)\Pi_\perp)^{-1}\Phi, (\Pi_\perp(H_0 - z)\Pi_\perp)^{-1}\Phi\rangle \tag{5.39}$$

$$= \int_{\sigma(\Pi_\perp H_0 \Pi_\perp)} \frac{1}{|\lambda - z|^2}\, \mathrm{d}\mu_\Phi(\lambda) \tag{5.40}$$

$$\leq \frac{1}{|E_1 - z|^2}\|\Phi\|^2. \tag{5.41}$$

For $|z + E_0| < \frac{|E_1+E_0|}{2}$ we get that

$$\|(\Pi_\perp(H_0 - z)\Pi_\perp)^{-1}\| = \frac{1}{|E_1 - z|} < \frac{2}{|E_1 + E_0|}. \tag{5.42}$$

This concludes the proof. □

We use the lemma to prove the following result.

Theorem 5.2.5 *Let $E_1 := \min \sigma(h_s)\setminus\{-E_0\}$, and let z satisfy $|z+E_0| < \frac{|E_1+E_0|}{2}$. Then there exists $C > 0$ such that*

$$[\Pi_\perp(H_\kappa - z)\Pi_\perp]^{-1} \tag{5.43}$$

exists and is an analytic function of κ when $|\kappa| < C$.

Proof. To simplify notation we denote by $H_{\perp,z} = \Pi_\perp(H_0 - z)\Pi_\perp$. Then we can write

$$\Pi_\perp(H_\kappa - z)\Pi_\perp = (\mathbb{1} + \kappa\Pi_\perp V\Pi_\perp H_{\perp,z}^{-1})H_{\perp,z}. \tag{5.44}$$

Taking the inverse of (5.44) we get

$$[\Pi_\perp(H_\kappa - z)\Pi_\perp]^{-1} = H_{\perp,z}^{-1}(\mathbb{1} + \kappa\Pi_\perp V\Pi_\perp H_{\perp,z}^{-1})^{-1}. \tag{5.45}$$

Equation (5.45) shows that the inverse of $\Pi_\perp(H_\kappa - z)\Pi_\perp$ exists if and only if $H_{\perp,z}^{-1}$ and $(\mathbb{1} + \kappa\Pi_\perp V\Pi_\perp H_{\perp,z}^{-1})^{-1}$ exists. By Lemma 5.2.4, we know that $H_{\perp,z}^{-1}$ exists and is bounded when z satisfies $|z + E_0| < \frac{|E_1+E_0|}{2}$. We want to apply Theorem A.1.6, to do that we need to show that there exists $\kappa > 0$ such that

$$\|\kappa\Pi_\perp V\Pi_\perp H_{\perp,z}^{-1}\| < 1. \tag{5.46}$$

By Equation (5.42) we see that the norm

$$\|\kappa\Pi_\perp V\Pi_\perp H_{\perp,z}^{-1}\| < \frac{|\kappa|2\|V\|}{|E_1 + E_0|}. \tag{5.47}$$

The type of interactions we have chosen implies that $\|V\| < \infty$. Then we get that (5.46) holds when

$$|\kappa| \leq \frac{|E_1 + E_0|}{2\|V\|}. \tag{5.48}$$

Since $|E_1 + E_0| > 0$ and $\|V\| < \infty$, we know that there exists such a $\kappa > 0$. Then the inverse of $\mathbb{1} + \kappa\Pi_\perp V\Pi_\perp H_{\perp,z}^{-1}$ exists and we can write it as a Neumann series

$$(\mathbb{1} + \kappa\Pi_\perp V\Pi_\perp H_{\perp,z}^{-1})^{-1} = \sum_{n=0}^{\infty}(-1)^n\kappa^n(\Pi_\perp V\Pi_\perp H_{\perp,z}^{-1})^n. \tag{5.49}$$

For κ satisfying (5.48), we have that

$$[\Pi_\perp(H_\kappa - z)\Pi_\perp]^{-1} = \sum_{n=0}^{\infty}\kappa^n A_n(z), \tag{5.50}$$

where

$$A_n(z) := (-1)^n H_{\perp,z}^{-1}(\Pi_\perp V\Pi_\perp H_{\perp,z}^{-1})^n. \tag{5.51}$$

Since we can write $[\Pi_\perp(H_\kappa - z)\Pi_\perp]^{-1}$ as a power series in κ it must be analytic in κ. □

If $|z + E_0| < \frac{|E_1+E_0|}{2}$ and $\kappa \leq \frac{|E_1+E_0|}{2\|V\|}$, then Theorem 5.2.5 and the Feshbach formula gives that the resolvent of H_κ exists if and only if the inverse of

$$\Pi(H_\kappa - z)\Pi - \Pi H_\kappa\Pi_\perp(\Pi_\perp(H_\kappa - z)\Pi_\perp)^{-1}\Pi_\perp H_\kappa\Pi \tag{5.52}$$

exists as an operator on $\Pi L^2(\mathbb{R}^2)$.

We will simplify or rewrite (5.52) a bit. By direct calculation, we see that

$$\Pi V \Pi = |\Psi\rangle \left(\int v\left(t - \frac{s'}{2}\right) \Psi(s')\, \mathrm{d}s' - \int v\left(t + \frac{s'}{2}\right) \Psi(s')\, \mathrm{d}s' \right) \langle \Psi| = 0, \quad (5.53)$$

since the eigenstate Ψ is even. Then we have $\Pi(H_\kappa - z)\Pi = \Pi(H_0 - z)\Pi$. Additionally, we know that $\Pi_\perp H_\kappa \Pi = -\kappa \Pi_\perp V \Pi$ and $\Pi H_\kappa \Pi_\perp = -\kappa \Pi V \Pi_\perp$, since Π and $\Pi_\perp$ commutes with H_0. Using this the operator in (5.52) simplifies to

$$\Pi(H_0 - z)\Pi - \kappa^2 \Pi V \Pi_\perp \left(\sum_{n=0}^{\infty} \kappa^n A_n(z) \right) \Pi_\perp V \Pi, \quad (5.54)$$

where $A_n(z)$ is given by (5.51). By direct calculations we can also see that

$$\Pi(H_0 - z)\Pi = (h_t - E_0 - z) \otimes P. \quad (5.55)$$

The operator in (5.52) can then be written as

$$(h_t - E_0 - z) \otimes P - \kappa^2 \Pi V \Pi_\perp \left(\sum_{n=0}^{\infty} \kappa^n A_n(z) \right) \Pi_\perp V \Pi, \quad (5.56)$$

on $\Pi L^2(\mathbb{R}^2)$. Thus, the only dependence on the variable s is from the eigenfunction $\Psi(s)$. Consequently, we can think of the operator (5.52) as a operator depending only on the variable t.

Let z and κ be as in Theorem 5.2.5, and assume that $|z + E_0| > C\kappa^2$ for some $C > 0$. We want to show that the inverse of the operator in (5.56) exists for all such z. By Theorem 3.1.3, we know that $(z + E_0) \in \rho(h_t)$. Theorem A.2.2 gives

$$\|(h_t - E_0 - z)^{-1}\| \leq \frac{1}{|E_0 + z|} < \frac{1}{C\kappa^2}. \quad (5.57)$$

Let $A := (h_t - E_0 - z)$, and define

$$B := -\Pi V \Pi_\perp \left(\sum_{n=0}^{\infty} \kappa^n A_n(z) \right) \Pi_\perp V \Pi. \quad (5.58)$$

Then the operator is $A + \kappa^2 B$, and the inverse can be written as

$$(A + \kappa^2 B)^{-1} = A^{-1}(\mathbb{1} + \kappa^2 B A^{-1})^{-1}. \quad (5.59)$$

Since A^{-1} exists, $(A + \kappa^2 B)^{-1}$ exists if $\|\kappa^2 B A^{-1}\| < 1$. But $\|B\| \leq K$ for some constant $K > 0$, and by Equation (5.57) the norm is

$$\|\kappa^2 B A^{-1}\| \leq \frac{K}{C}. \quad (5.60)$$

Choosing $C > K$, we find that the inverse of the operator in (5.56) exists. By the

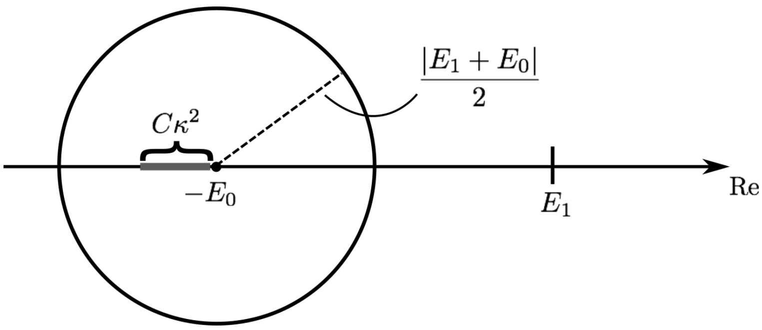

Figure 5.1: Illustration of the area in which we look for eigenvalues

discussion above, we know a priori to look for eigenvalues of H_κ in

$$|z + E_0| \le C\kappa^2, \tag{5.61}$$

for some $C > 0$. The situtation is illustrated in Figure 5.1. We can write the operator in (5.56) as

$$-\frac{1}{4}\frac{\partial^2}{\partial t^2} - E_0 - z - \kappa^2 \Pi V \Pi_\perp A_0(-E_0)\Pi_\perp V \Pi + \mathcal{O}(\kappa^4), \tag{5.62}$$

since the error we get by using $-E_0$ instead of z in the sum (5.49) is of order κ^2. Finally, by using the definition of $A_n(z)$ we see that the operator in (5.52) can be expressed as

$$-\frac{1}{4}\frac{\partial^2}{\partial t^2} - E_0 - z - \kappa^2 \Pi V \Pi_\perp [\Pi_\perp (H_0 + E_0)\Pi_\perp]^{-1} \Pi_\perp V \Pi + \mathcal{O}(\kappa^4). \tag{5.63}$$

Let us define by $B_0 := -\frac{1}{4}\frac{\partial^2}{\partial t^2} - E_0$ and

$$B_1 := \Pi V \Pi_\perp [\Pi_\perp (H_0 + E_0)\Pi_\perp]^{-1} \Pi_\perp V \Pi. \tag{5.64}$$

Then the operator in (5.63) is $B_0 - \kappa^2 B_1 + \mathcal{O}(\kappa^4)$. We can consider the term $\mathcal{O}(\kappa^4)$ as a perturbation of the operator $B_0 - \kappa^2 B_1$. In the next section we use the Birman-Schwinger principle to show that $B_0 - \kappa^2 B_1$ has an eigenvalue in the interval $[-E_0 - C\kappa^2, -E_0)$.

5.3 Eigenvalues of $B_0 - \kappa^2 B_1$ in $[-E_0 - C\kappa^2, -E_0)$

In this section, we use something called the Birman-Schwinger principle to show that the operator $B_0 - \kappa^2 B_1$ has an eigenvalue in the interval $[-E_0 - C\kappa^2, -E_0)$. Furthermore, we show that the leading behavior of the eigenvalue is κ^4. For information on the Birman-Schwinger principle, we refer to [Simon, 1971]. The approach we take in this section is quite similar to that of Section 4.2.

Note that the operator B_1 in (5.64) can be written as $B_1 = W^*W$, where

$$W = [\Pi_\perp(H_0 + E_0)\Pi_\perp]^{-\frac{1}{2}}\Pi_\perp V\Pi. \tag{5.65}$$

This leads to the first result of this section.

Theorem 5.3.1 *Let $B_0 - \kappa^2 B_1$ be the operator defined in the Section 5.2, and write $B_1 = W^*W$, where W is given by (5.65). Then $E \in [-E_0 - C\kappa^2, -E_0)$ is an eigenvalue of $B_0 + \kappa^2 B_1$ if and only if*

$$\mathbb{1} - \kappa^2 W(B_0 - E)^{-1}W^* \tag{5.66}$$

is singular.

Proof. Let $E \in [-E_0 - C\kappa^2, -E_0)$, and write

$$B_0 - \kappa^2 B_1 - E = (\mathbb{1} - \kappa^2 B_1(B_0 - E)^{-1})(B_0 - E). \tag{5.67}$$

The operator $(B_0 - E)^{-1}$ exists, since $E \in \rho(B_0)$. Then

$$(B_0 - \kappa^2 B_1 - E)^{-1} = (B_0 - E)^{-1}(\mathbb{1} - \kappa^2 B_1(B_0 - E)^{-1})^{-1}. \tag{5.68}$$

Thus E is an eigenvalue of $B_0 - \kappa^2 B_1$ if and only if $\mathbb{1} - \kappa^2 B_1(B_0 - E)^{-1}$ is singular. Using similar calculations as in the previous section, we could show that κ can be choosen sufficiently small, such that

$$\kappa^2 \|B_1(B_0 - E)^{-1}\| < 1. \tag{5.69}$$

Then we expand in a Neumann series and find

$$\mathbb{1} - \kappa^2 B_1(B_0 - E)^{-1} = \sum_{n=0}^{\infty}(-1)^n[\kappa^2 B_1(B_0 - E)^{-1}]^n. \tag{5.70}$$

Inserting (5.70) in (5.68) and using that $B_1 = W^*W$, we rewrite (5.68) in a similar fashion to what we did in Section 4.2 to get

$$\begin{aligned}(B_0 - \kappa^2 B_1 - E)^{-1} = (B_0 - E)^{-1} - \kappa^2(B_0 - E)^{-1}W^* \\ \times \left[\mathbb{1} - \kappa^2 W(B_0 - E)^{-1}W^*\right]^{-1} W(B_0 - E)^{-1}.\end{aligned} \tag{5.71}$$

Consequently, we know that $E \in [-E_0 - C\kappa^2, -E_0)$ is an eigenvalue of $B_0 + \kappa^2 B_1$, if and only if

$$\mathbb{1} - \kappa^2 W(B_0 - E)^{-1}W^* \tag{5.72}$$

is singular. □

The relation between the singularity of (5.66) and the eigenvalues of $B_0 - \kappa^2 B_1$ is what is typically called the Birman-Schwinger principle. In the next result we use the Birman-Schwinger principle and Feshbachs formula to determine the eigenvalue of $B_0 - \kappa^2 B_1$.

Theorem 5.3.2 *Let $B_0 - \kappa^2 B_1$ be the operator defined in the Section 5.2 and write $B_1 = W^* W$, where W is given by* (5.65). *Assume that the integral kernel of W satisfies*

$$W(t,t') \le C_0 e^{-|t|} e^{-|t'|}, \qquad C_0 > 0. \tag{5.73}$$

Then $B_0 - \kappa^2 B_1$ has an eigenvalue $E \in [-E_0 - C\kappa^2, -E_0)$.

Proof. By Theorem 5.3.1, we can determine the eigenvalues E of $B_0 - \kappa^2 B_1$ in $[-E_0 - C\kappa^2, -E_0)$ by considering when the operator in (5.66) is singular.

Define $E' := E_0 + E < 0$, then there exists $\lambda \in \mathbb{C}$ with $\operatorname{Im}\lambda > 0$ and $\operatorname{Re}\lambda = 0$ such that $E' = \lambda^2$. Then we cam write (5.66) as

$$\mathbb{1} - 4\kappa^2 W \left(-\frac{\partial^2}{\partial t^2} - 4\lambda^2 \right)^{-1} W^*. \tag{5.74}$$

The integral kernel of the free resolvent in one-dimension is given by

$$G_0(x,y,\lambda) = \frac{1}{2|\lambda|} e^{-|\lambda||x-y|}. \tag{5.75}$$

From similar considerations as in the proof of Theorem 4.2.3, we can show that the operator in (5.74) has an integral kernel given by

$$\mathbb{1} - \frac{\kappa^2}{|\lambda|} \iint W(t,x) e^{-2|\lambda||x-y|} W(y,t') \,\mathrm{d}x\,\mathrm{d}y. \tag{5.76}$$

We want to determine the values, for which the integral kernel is zero. To do this, we use the following identity to rewrite the integral kernel

$$e^{-s} = 1 - s\int_0^s e^{-t}\,\mathrm{d}t. \tag{5.77}$$

Inserting (5.77) in (5.76) we get

$$\mathbb{1} - \frac{\kappa^2}{|\lambda|} \iint W(t,x) W(y,t') \,\mathrm{d}x\,\mathrm{d}y + \kappa^2 B_3(|\lambda|, t, t'), \tag{5.78}$$

where

$$B_3(|\lambda|, t, t') := 2 \iint W(t,x) \int_0^{|x-y|} e^{-2|\lambda| s} W(y,t') \,\mathrm{d}s\,\mathrm{d}y\,\mathrm{d}x. \tag{5.79}$$

We would like to apply Feshbachs formula to (5.78). To do this, we need an orthogonal projection operator. We define the rank-1 projection P, which acts on $\phi \in L^2(\mathbb{R})$ by

$$\frac{1}{K} \int W(t,x)\,\mathrm{d}x \int \left(\int W(y,t')\,\mathrm{d}y \right) \phi(t')\,\mathrm{d}t', \tag{5.80}$$

where K is the constant given by

$$K := \int \left(\int W(t,x)\,\mathrm{d}x \right) \left(\int W(y,t)\,\mathrm{d}y \right) \mathrm{d}t. \tag{5.81}$$

Then the integral kernel in (5.78) is

$$\mathbb{1} - \frac{\kappa^2 K}{|\lambda|} P + \kappa^2 B_3(|\lambda|, t, t'). \tag{5.82}$$

It is easy to show that P is actually an orthogonal projection, and so it can be used with Feshbachs formula. Defining $P_\perp := \mathbb{1} - P$, we see that

$$P_\perp \left(\mathbb{1} - \frac{\kappa^2 K}{|\lambda|} P + \kappa^2 B_3(|\lambda|, t, t') \right) P_\perp = P_\perp (\mathbb{1} + \kappa^2 B_3(|\lambda|, t, t')) P_\perp \tag{5.83}$$

We show that the right-hand side is invertible. By the Schur test in Theorem 4.1.1, we have

$$\begin{aligned} \|\kappa^2 B_3(|\lambda|, t, t')\| &\leq 2\kappa^2 \sup_{t' \in \mathbb{R}} \int B_3(|\lambda|, t, t') \, \mathrm{d}t \qquad (5.84) \\ &\leq 2\kappa^2 \sup_{t' \in \mathbb{R}} \iiint \left| W(t, x) \int_0^{|x-y|} e^{-2|\lambda| s} \overline{W(y, t')} \, \mathrm{d}s \right| \mathrm{d}x \, \mathrm{d}y \, \mathrm{d}t. \end{aligned}$$

We use the following identity to rewrite (5.84),

$$\int_0^x e^{-s} \, \mathrm{d}s = 1 - e^{-x} \leq x. \tag{5.85}$$

Applying the identity to (5.84), we find

$$\|\kappa^2 B_3(|\lambda|, t, t')\| \leq 2\kappa^2 \sup_{t' \in \mathbb{R}} \iiint W(t, x)(|x| + |y|) \overline{W(y, t')} \, \mathrm{d}x \, \mathrm{d}y \, \mathrm{d}t. \tag{5.86}$$

Using the assumption about the behavior of $W(t, t')$ from (5.73), we get

$$\|\kappa^2 B_3(|\lambda|, t, t')\| \leq 2\kappa^2 C^2 \iiint e^{-|t|} e^{-|x|} (|x| + |y|) e^{-|y|} \, \mathrm{d}x \, \mathrm{d}y \, \mathrm{d}t \tag{5.87}$$

$$= 32\kappa^2 C^2, \qquad C > 0. \tag{5.88}$$

Consequently, we can choose κ such that the right-hand side of (5.83) is invertible. Then Feshbachs formula gives that the values for which (5.74) is singular, is the $E' = \lambda^2$ which satisfies

$$\mathbb{1} - \frac{\kappa^2 K}{|\lambda|} + \kappa^2 B_3(|\lambda|, t, t') + \mathcal{O}(\kappa^4) = 0, \tag{5.89}$$

where the term $\mathcal{O}(\kappa^4)$ term corresponds to $W(z)$ defined in (5.8). Multiplying by $|\lambda|$ we find

$$|\lambda| - \kappa^2 K + \kappa^2 |\lambda| B_3(|\lambda|, t, t') + \mathcal{O}(\kappa^4, |\lambda|) = 0. \tag{5.90}$$

Let us define the function

$$\mathcal{F}\left(\lambda, \kappa^2\right) := \lambda - \kappa^2 K + \kappa^2 \lambda B_3(\lambda, t, t') + \mathcal{O}(\kappa^4, \lambda). \tag{5.91}$$

We want to use the implicit function theorem, Theorem 9.28 in [Rudin, 1976], on $\mathcal{F}(\lambda, \kappa^2)$. Note that $\mathcal{F}(0,0) = 0$. To apply the implicit function theorem we need to show that $\mathcal{F} \in C^1$, and that

$$\left.\frac{\partial \mathcal{F}(\lambda, \kappa^2)}{\partial \lambda}\right|_{\kappa^2=0,\lambda=0} \neq 0, \quad \text{and} \quad \left.\frac{\partial \mathcal{F}(\lambda, \kappa^2)}{\partial \kappa^2}\right|_{\kappa^2=0,\lambda=0} \neq 0. \tag{5.92}$$

It is obvious that the first order partial derivatives exists, and that (5.92) holds. By considering $B_3(\lambda, t, t')$ and the remainder term $\mathcal{O}(\kappa^4, \lambda)$, we could show that the second order partial derivatives exists, and thus $\mathcal{F} \in C^1$. The implicit function theorem implies that there exists an open subset about $(0,0)$, where

$$\lambda = \kappa^2 K - \kappa^2 \lambda B_3(\lambda, t, t') - \mathcal{O}(\kappa^4, \lambda). \tag{5.93}$$

Squaring both sides, and taking $\lambda^2 = E'$ shows that (5.74) is singular for an $E' \in [-C\kappa^2, 0)$, and thus there exist an eigenvalue $E \in [-E_0 - C\kappa^2, -E_0)$ of $B_0 - \kappa^2 B_1$. □

We have a few remarks to the previous theorem and proof.

The first remark is that the assumption in (5.77) is stronger than necessary. What is actually needed, is simply that the decay of $W(t,t')$ allows choosing a κ such that

$$\|\kappa^2 B_3(\sqrt{E'}, t, t')\| < 1. \tag{5.94}$$

Additionally, we have not actually shown that such a decay property hold for the integral kernel of W, where W is given by (5.65). But we expect that this indeed is the case.

The second remark is that Equation (5.93) implies that the eigenvalue E of $B_0 - \kappa^2 B_1$ behaves like $\mathcal{O}(\kappa^4)$. Unfortunately this has the consequence that we cannot be sure the operator $B_0 - \kappa^2 B_1 + \mathcal{O}(\kappa^4)$ has an eigenvalue with behavior $\mathcal{O}(\kappa^4)$, since the error term is $\mathcal{O}(\kappa^4)$ aswell. To solve this problem we return to the operator in (5.56), recall that it is given by

$$B_0 - z - \kappa^2 \Pi V \Pi_\perp \left(\sum_{n=0}^{\infty} \kappa^n A_n(z) \right) \Pi_\perp V \Pi, \tag{5.95}$$

where $B_0 = -\frac{1}{4}\frac{\partial^2}{\partial t^2} - E_0$. We still know that any eigenvalue E of H_κ must atleast satisfy $-E_0 - C\kappa^2 \leq E < -E_0$, for some constant $C > 0$. So we write

$$B_0 - z - \kappa^2 \Pi V \Pi_\perp \left(A_0(z)\right) \Pi_\perp V \Pi + \mathcal{O}(\kappa^5). \tag{5.96}$$

Writing

$$A_0(z) = A_0(-E_0) + (z + E_0)\tilde{A}_0(-E_0, z), \tag{5.97}$$

where $\tilde{A}_0(-E_0, z)$ is an operator determined by expanding $A_0(z)$ around $z = -E_0$. The operator in (5.96) is

$$B_0 - z - \kappa^2 B_1 + \mathcal{O}(\kappa^2(z + E_0)) + \mathcal{O}(\kappa^5). \tag{5.98}$$

But we have already determined that the eigenvalue E of $B_0 - \kappa^2 B_1$ behaves like $\mathcal{O}(\kappa^4)$. Thus, for $z = E$ in (5.98), we find

$$B_0 - z - \kappa^2 B_1 + \mathcal{O}(\kappa^6) + \mathcal{O}(\kappa^5) = B_0 - z - \kappa^2 B_1 + \mathcal{O}(\kappa^5). \tag{5.99}$$

Now the eigenvalue cannot be cancelled by the error term, since that term now behaves like $\mathcal{O}(\kappa^5)$. Finally, we conclude that the original system represented by H_κ in (5.1) has a discrete eigenvalue in the interval $[-E_0 - C_\kappa \kappa^4, -E_0)$ for sufficiently small κ and a constant $C_\kappa > 0$.

Chapter 6

Recapitulation

The thesis is concluded by a short recapitulation of the work done during the project and some suggestions for future work.

In Chapter 2 a Schrödinger operator describing the systems consisting of three particles with Dirac delta interactions was constructed, and the domain of the operator was described in detail. This served as the foundation for a study of the essential spectrum of the operator, which was determined using the HVZ theorem in Chapter 3. In Chapter 4 preliminary results for the determination of the existence of discrete eigenvalues of the system was shown. The actual determination of any discrete eigenvalues was abandoned after it was suggested we consider perturbation theory for the system in Chapter 5 instead. In Chapter 5 a system, which might be interpreted as an exciton in the vicinity of a positively charged nucleus in a one-dimensional semi-conductor, was considered. The existence of a discrete eigenvalue of the perturbed system was shown. Furthermore, the behavior of the eigenvalue as a function of the coupling constant κ was shown to be $\mathcal{O}(\kappa^4)$. The existence and the behavior of the eigenvalue were shown under the assumption of certain decay properties, as mentioned at the end of Section 5.3.

6.1 Future Work

Due to the time constraint it was not possible to adress all the problems that was encountered in the project. These problems could be addressed in future work. The first obvious problem would be to show whether the integral kernel of (5.65) actually does satisfy the decay conditions that was assumed. And if it does not satisfy these decay conditions, then decide whether another type of interaction v could be chosen such that integral kernel does satisfy the decay conditions. It would also be interesting to try and show the existence and the behavior of a discrete eigenvalue in the case where the system has Dirac delta particle interactions.

Appendix A

Miscellaneous Results

In this appendix we have collected results and definitions, which are used throughout the report. The results are mainly included to keep the report as self-contained as possible. Some of the results are stated without proof, but references to books or papers containing proofs will be supplied. Most of the results are from [Kreyszig, 1978], [Reed and Simon, 1980] and [Reed and Simon, 1975].

A.1 Operator on Hilbert Spaces

In this section we present relevant results about unbounded operators on Hilbert spaces, and argue why they are to be defined on dense subspaces. We begin by defining the adjoint of a possible unbounded operator.

Definition A.1.1
Let T be an operator in $\mathcal{H}$, where $\mathcal{H}$ is a complex Hilbert space, with $D(T)$ dense in $\mathcal{H}$. Let $D(T^*)$ be the set of $y \in \mathcal{H}$ such that there exists $y^* \in \mathcal{H}$ which satisfies

$$\langle y, Tx \rangle = \langle y^*, x \rangle, \quad \forall x \in D(T). \tag{A.1}$$

Then T^*, the adjoint operator of T, is the operator which satisfies $T^*y = y^*$ for $y \in D(T^*)$.

We state the following theorem.

Theorem A.1.2 *Let $\mathcal{H}$ be a Hilbert space, and Y a closed subspace of $\mathcal{H}$. Then*

$$\mathcal{H} = Y \oplus X, \tag{A.2}$$

where $X = Y^{\perp}$.

Proof. A proof is available in Theorem 3.3-4 in [Kreyszig, 1978]. □

Note, that the adjoint operator is only defined for operators which are densely defined in $\mathcal{H}$, there is an important reason for this choice of definition. For T^* to be a well defined operator we must have that y^* is unique for each $y \in D(T^*)$.

Theorem A.1.3 *Let T be an unbounded operator, and let T^* be the adjoint of T. Then T^* is a well defined operator, if and only if $D(T)$ is dense in $\mathcal{H}$.*

Proof. Assume that $D(T)$ is not dense in $\mathcal{H}$. Then $\overline{D(T)} \neq \mathcal{H}$, and by Theorem A.1.2 there exists a nonzero element $y_0 \in \mathcal{H}$ such that $\langle y_0, x\rangle = 0$ for all $x \in D(T)$. But then

$$\langle y^*, x\rangle = \langle y^*, x\rangle + \langle y_0, x\rangle = \langle y^* + y_0, x\rangle, \tag{A.3}$$

and T^* is not well defined.

Conversely assume that $D(T)$ is dense in H. Then $\langle x, y_0\rangle = 0$ for all $x \in D(T)$ implies that $y_0 = 0$, and we have that y^* is unique and T^* is well defined. □

We now give the definition of a densely defined self-adjoint operator.

Definition A.1.4
Let $T : D(T) \to \mathcal{H}$ be a linear operator, and let $D(T)$ be dense in $\mathcal{H}$. Then T is said to be self-adjoint if $D(T) = D(T^*)$ and $Ty = T^*y$ for all $y \in D(T)$.

Now follows a few results regarding bounded operators. The first of these results is Riesz representation theorem. The Riesz representation theorem is used especially in Chapter 2.

Theorem A.1.5 (Riesz Representation) *Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be Hilbert spaces, and $Q : \mathcal{H}_1 \times \mathcal{H}_2 \to \mathbb{C}$ a bounded sesquilinear form. Then Q has a representation as*

$$Q(x, y) = \langle x, Sy\rangle, \tag{A.4}$$

where $S : H_2 \to H_1$. The operator S is uniquely defined by Q, and has norm $\|S\| = \|Q\|$.

Proof. A proof is available in Theorem 3.8-4 in [Kreyszig, 1978]. □

The next result regards the inverse of a bounded operator.

Theorem A.1.6 *Let $T : \mathcal{H} \to \mathcal{H}$, where $\mathcal{H}$ is a Banach space. Assume that T is bounded. If $\|T\| < 1$, then $(\mathbb{1} - T)^{-1}$ as a bounded operator on all of $\mathcal{H}$, and can be expanded in a Neumann series, as*

$$(\mathbb{1} - T) = \sum_{j=0}^{\infty} T^j. \tag{A.5}$$

Proof. A proof is available in Theorem 7.3-1 in [Kreyszig, 1978]. □

A.2 Spectrum, Spectral Theorem and Resolvent Properties

In this section we present various results regarding the spectrum, the spectral theorem and the resolvent operator.

The following equation is called the first resolvent equation. Let A be a linear operator, and let $z, w \in \rho(A)$. Then the first resolvent equation is

$$R_A(z) - R_A(w) = (z - w)R_A(z)R_A(w), \tag{A.6}$$

where $R_A(z)$ is the resolvent of A.

Theorem A.2.1 (Spectral Theorem) *Let A be a self-adjoint operator. Then there exists a unique projection-valued measure P_A such that*

$$A = \int_{\mathbb{R}} \lambda \, dP_A(\lambda). \tag{A.7}$$

If $f(\cdot)$ is a real-valued measurable function on $\mathbb{R}$, then $f(A)$ defined by

$$f(A) = \int_{-\infty}^{\infty} f(\lambda) \, dP_A(\lambda), \tag{A.8}$$

is a self-adjoint operator on

$$D_f = \left\{ \phi : \int_{-\infty}^{\infty} |f(\lambda)|^2 \, d(\phi, P_A(\lambda)\phi) < \infty \right\}. \tag{A.9}$$

Proof. A thorough proof of the spectral theorem is given in Chapter VII and in Section VIII.3 in [Reed and Simon, 1980]. □

Equation (A.8) is to be understood as the operator defined by the form

$$\langle \phi, f(A)\phi \rangle = \int_{\sigma(A)} f(\lambda) \, \mathrm{d}(\phi, P_A(\lambda)\phi). \tag{A.10}$$

We will sometimes write $\mathrm{d}(\phi, P_A(\lambda)\phi) = \mathrm{d}\mu_\phi(\lambda)$ for the spectral measure. From the spectral theorem we can get a bound for the operator norm of the resolvent.

Theorem A.2.2 *Let A be a self-adjoint operator on a Hilbert space $\mathcal{H}$, and let $z \in \rho(A)$. Then*

$$\|(A - z)^{-1}\| \leq \frac{1}{\mathrm{dist}(z, \sigma(A))}, \tag{A.11}$$

where $\mathrm{dist}(z, \sigma(A)) = \inf_{x \in \sigma(A)} |z - x|$.

Proof. Consider a self-adjoint operator A on $\mathcal{H}$, and let $z \in \rho(A)$. If $\psi \in \mathcal{H}$, then

$$\|(A-z)^{-1}\psi\|^2 = \langle (A-z)^{-1}\psi, (A-z)^{-1}\psi\rangle = \langle \psi, (A-z)^{-2}\psi\rangle, \qquad \text{(A.12)}$$

since the resolvent operator of a self-adjoint operator is self-adjoint. The spectral theorem gives

$$\langle \psi, (A-z)^{-2}\psi\rangle = \int_{\sigma(A)} \frac{1}{|\lambda - z|^2}\, \mathrm{d}\mu_\psi(\lambda) \qquad \text{(A.13)}$$

$$\leq \sup_{\lambda\in\sigma(A)} \frac{1}{|\lambda - z|^2} \int \mathrm{d}\mu_\psi(\lambda) \qquad \text{(A.14)}$$

$$= \sup_{\lambda\in\sigma(A)} \frac{1}{|\lambda - z|^2} \|\psi\|^2. \qquad \text{(A.15)}$$

Consequently $\|(A-z)^{-1}\|^2 \leq \sup_{\lambda\in\sigma(A)} \frac{1}{|\lambda-z|^2}$. Which concludes the proof. □

An obvious corollary to the previous theorem is

Theorem A.2.3 *Let A be a self-adjoint operator on a Hilbert space $\mathcal{H}$, and let $z = x + iy \in \mathbb{C}$. If $y \neq 0$ then*

$$\|(A-z)^{-1}\| \leq \frac{1}{|y|} \qquad \text{(A.16)}$$

We now state Stone's formula which we will use to prove the HVZ theorem and the Helffer-Sjöstrand formula.

Theorem A.2.4 (Stone's Formula) *Let A be a self-adjoint operator on a Hilbert space $\mathcal{H}$. Then*

$$\frac{1}{2}(P_A([a,b]) + P_A((a,b))) = \operatorname*{s-lim}_{\epsilon\downarrow 0} \frac{1}{2\pi i}\int_a^b [R_A(\lambda - i\epsilon) - R_A(\lambda + i\epsilon)]\ d\lambda. \qquad \text{(A.17)}$$

Proof. A proof is available in Theorem VII.13 in [Reed and Simon, 1980]. □

By the Spectral theorem and Stone's formula we can write

$$f(A) = \operatorname*{s-lim}_{\epsilon\downarrow 0} \frac{1}{2\pi i}\int_a^b f(\lambda)\, [R_A(\lambda - i\epsilon) - R_A(\lambda + i\epsilon)]\ \mathrm{d}\lambda, \qquad \text{(A.18)}$$

for a real measurable function on $[a, b]$.

Theorem A.2.5 *Let A be a self-adjoint operator on a Hilbert space $\mathcal{H}$, and let P_A be the corresponding projection-valued measure given by the spectral theorem. Then the spectrum of A is given by*

$$\sigma(A) = \{\lambda \in \mathbb{R} : P_A((\lambda - \epsilon, \lambda + \epsilon) \neq 0), \quad \forall \epsilon > 0\}. \qquad \text{(A.19)}$$

The previous theorem motivates the decomposition of the spectrum into a discrete spectrum and an essential spectrum, which are defined in the following definition.

Definition A.2.6
Let A be a self-adjoint operator. The discrete spectrum $\sigma_d(A)$ is the set

$$\sigma_d(A) = \{\lambda \in \sigma(A) : \exists \epsilon > 0, \ s.t. \ \operatorname{rank} P_A((\lambda - \epsilon, \lambda + \epsilon)) < \infty\}. \tag{A.20}$$

By rank *we mean the dimension of the range. The essential spectrum is defined to be $\sigma_{ess}(A) = \sigma(A) \setminus \sigma_d(A)$.*

By the definition of the discrete spectrum, it is obvious that the essential spectrum must be equal to the set

$$\sigma_{ess}(A) = \{\lambda \in \sigma(A) : \operatorname{rank} P_A((\lambda - \epsilon, \lambda + \epsilon)) = \infty, \quad \forall \epsilon > 0\}. \tag{A.21}$$

A.3 Function Spaces

In this section multi-index notation is used. Multi-index notation is described on p. 133 in [Reed and Simon, 1980]. We introduce the Schwartz space and the space of tempered distributions.

Definition A.3.1
Let $f : \mathbb{R}^n \to \mathbb{C}$ and $f \in C^\infty$. Define the seminorm

$$\|f\|_{\alpha,\beta} \equiv \sup_{x \in \mathbb{R}^n} |x^\alpha D^\beta f(x)|. \tag{A.22}$$

The Schwartz space on $\mathbb{R}^n$ is the space of functions

$$\mathscr{S}(\mathbb{R}^n) = \left\{ f \in \mathbb{C}^\infty : \|f\|_{\alpha,\beta} < \infty \quad \forall \alpha, \beta \in I_+^n \right\}, \tag{A.23}$$

where I_+^n is the set of n-tuples of nonnegative integers. The Schwartz space is also called the space of rapidly decreasing functions.

The dual space of $\mathscr{S}(\mathbb{R}^n)$, which is denoted by $\mathscr{S}'(\mathbb{R}^n)$, is called the space of tempered distributions.

Next we introduce Sobolev spaces and the Sobolev embedding theorem. The Sobolev spaces are introduced since the domain of the Schrödinger operators we consider are Sobolev spaces.

Definition A.3.2
Let $f \in \mathscr{S}'(\mathbb{R}^n)$. Then f is said to be in the m'th Sobolev space if $\hat{f}$ is measurable and

$$\|f\|_{H^m}^2 = \int_{\mathbb{R}^n} (1 + |k|^2)^m |\hat{f}(k)|^2 \, dk < \infty. \tag{A.24}$$

The m'th Sobolev space on $\mathbb{R}^n$ is denoted by $H^m(\mathbb{R}^n)$.

Note that $f \in H^m(\mathbb{R}^n)$ is equivalent to $(1+|k|^2)^{m/2}\hat{f} \in L^2(\mathbb{R}^n)$. The following theorem gives an alternative definition of the Sobolev spaces.

Theorem A.3.3 *Let $m \in \mathbb{N}$, then $f \in H^m(\mathbb{R}^n)$ if and only if $D^\alpha(f) \in L^2(\mathbb{R}^n)$ for all $|\alpha| \leq m$.*

Proof. Assume that $f \in H^m(\mathbb{R}^n)$ for some $m \in \mathbb{N}$. We have that $D^\alpha(f) = (ik)^\alpha \hat{f}$ for all $f \in \mathscr{S}'(\mathbb{R}^n)$. If $|\alpha| \leq m$ then $(ik)^\alpha \hat{f} \in L^2(\mathbb{R}^n)$ by the definition of the Sobolev spaces. By Plancherel's theorem we have that $D^\alpha(f) \in L^2(\mathbb{R}^n)$ for all $|\alpha| \leq m$.

Conversely, assume that $D^\alpha(f) \in L^2(\mathbb{R}^n)$ for all $|\alpha| \leq m$. Then $(ik)^\alpha \hat{f} \in L^2(\mathbb{R}^n)$ by Plancherel's theorem. But then $f \in H^m(\mathbb{R}^n)$. $\square$

Note that $D^\alpha(f)$ is in the sense of distributions.

The next result regarding Sobolev spaces is called Sobolev's Lemma and is a special case of Sobolev's embedding theorem.

Theorem A.3.4 (Sobolev's Lemma) *Let $f \in H^m(\mathbb{R}^n)$, where $m > n/2$. Also let $l \in \mathbb{N}_0$ satisfy $l < m - n/2$. Then $f \in C^l(\mathbb{R}^n)$.*

Proof. We prove the theorem for $n = 1$ to simplify notation, then $m > 1/2$. Since $f \in H^m(\mathbb{R})$ we have that

$$(1+|k|^2)^{m/2}\hat{f}(k) \in L^2(\mathbb{R}). \tag{A.25}$$

We also know that $(1+|k|^2)^{-1/4-\varepsilon} \in L^2(\mathbb{R})$ for all $\varepsilon > 0$. Thus from the Hölder inequality we have that

$$(1+|k|^2)^{m/2-1/4-\varepsilon}\hat{f}(k) \in L^1(\mathbb{R}). \tag{A.26}$$

This implies that for all $0 \leq \alpha \leq l$ we have the inequality

$$|k^\alpha \hat{f}(k)| \leq |k|^l (1+|k|)^{-m/2+1/4+\varepsilon} G(k), \tag{A.27}$$

for some $g(k) \in L^1(\mathbb{R})$. Actually $g(k) = (1+|k|^2)^{m/2-1/4-\varepsilon}\hat{f}(k)$. Since we can choose $\varepsilon > 0$ such that $l < m - 1/2 - 2\varepsilon$ we see that

$$|k|^l (1+|k|^2)^{-m/2+1/4+\varepsilon} \leq C, \tag{A.28}$$

for some constant $C > 0$. Then $k^\alpha \hat{f}(k) \in L^1(\mathbb{R})$ for all $0 \leq \alpha \leq l$.

Suppose that $l = 0$, then we just have to show that f is continuous. But

$$f(x) = \frac{1}{\sqrt{2\pi}} \int e^{ikx} \hat{f}(k)\, \mathrm{d}k, \tag{A.29}$$

and it follows from Lebesgue's dominated convergence theorem that

$$f(x+h) - f(x) = \frac{1}{\sqrt{2\pi}} \int e^{ikx}(e^{ikh} - 1)\hat{f}(k)\,\mathrm{d}k \tag{A.30}$$

goes toward zero for $h \to 0$.

Suppose instead that $l \geq 1$. Then

$$\begin{aligned} \frac{f(x+h) - f(x)}{h} &= \frac{1}{\sqrt{2\pi}} \int \frac{e^{ikx}}{h}(e^{ikh} - 1)\hat{f}(k)\,\mathrm{d}k \qquad \text{(A.31)} \\ &= \frac{1}{\sqrt{2\pi}} \int \frac{e^{ikx}}{h}(e^{ikh} - 1 + ikh - ikh)\hat{f}(k)\,\mathrm{d}k \\ &= \frac{1}{\sqrt{2\pi}} \int \frac{e^{ikx}}{h}(e^{ikh} - 1 - ikh)\hat{f}(k)\,\mathrm{d}k + \frac{1}{\sqrt{2\pi}} \int e^{ikx} ik\hat{f}(k)\,\mathrm{d}k \end{aligned}$$

But by Lebesgue's dominated convergence theorem we have that the first term in the final equality goes to zero. We see that $f \in C^1$. To show that $f \in C^l$ we note that $(1 + |k|^l)|\hat{f}(k)| \in L^1(\mathbb{R})$ and we can repeat the process of showing the existence of a derivative l times. □

We also have a need for the next result in Chapter 2.

Theorem A.3.5 *Let Ω be an arbitrary open subset of $\mathbb{R}^d$. Then $C^\infty(\Omega) \cap H^s(\Omega)$ is dense in $H^s(\Omega)$.*

Proof. We refer to the proof of proposition 2.12 in [Demengel and Demengel, 2007]. □

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