TWO-PARTICLE SCHRÖDINGER OPERATORS WITH POINT INTERACTIONS

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ABSTRACT

TWO-PARTICLE SCHRÖDINGER OPERATORS WITH POINT INTERACTIONS

In this thesis, a singular quantum mechanical problem, where two particles interact with each other through Dirac delta potentials in the plane, has been considered. The proof for the existence of a self-adjoint Hamiltonian operator for the model is given by using some operator theory techniques and renormalization idea in quantum field theory. Moreover, some necessary background for unbounded operators is reviewed in order to make the thesis as self-contained as possible.

ÖZET

NOKTASAL ETKİLEŞİM İÇEREN İKİ-PARÇACIKLI SCHRÖDINGER İŞLEMCİLERİ

Bu tezde, iki parçacığın düzlemde birbirleriyle Dirac delta potensiyeliyle etkileştiği tekil bir kuantum mekaniği problemi ele alınmıştır. Bazı operator teorisi teknikleri ve Kuantum alan teorisindeki renormalizasyon fikri kullanılarak, model için kendine eşlenik bir Hamiltoniyen operatünün var olduğunun ispatı verilmiştir. Ayrıca, tezin sadece kendi başına yeterli olabilmesi amacıyla, sınırlı olmayan operatörler için bazı gerekli olan alt yapı derlenecektir.

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LIST OF SYMBOLS

$\mathbb{N} = \{1, 2, 3, \dots\}$

$\mathbb{N}_0 = \{0, 1, 2, 3, \dots\}$

$\mathcal{H}$: Hilbert space

$\langle \cdot, \cdot \rangle$: Inner product

z: Complex number

$\mathrm{Im(z)}$: Imaginary part of z

$L^2(\mathbb{R}^n)$: Space of square integrable functios

$C_c(\mathbb{R}^n)$: Space of compactly supported functions

$C^\infty(\mathbb{R}^n)$: Space of smooth functions

$C_c^\infty(\mathbb{R}^n)$: Space of compactly supported smooth functions

$S(\mathbb{R}^n)$: Schwartz space

$\mathbb{P}_\psi$: Projection operator on ψ

X: Position operator

P: Momentum operator

Δ: Laplacian operator

$D(T)$: Domain of operators

$Ker(T)$: Kernel of operators

$Ran(T)$: Range of operators

$\Gamma(T)$: Graph of operators

$\subseteq$: Subspace or restriction (Depends on context)

$C^0[0, 1]$: Space of continuous functions

$C^1[0, 1]$: Space of once continuously differentiable functions

T^*: Adjoint of operators

$\overline{T}$: Closure of operator

π_1, π_2: Projection maps

$\dot{+}$: Orthogonal sum of spaces

$\oplus$: Direct sum of spaces

$\pi(T)$: Set of regular points of T

The end of a proof is shown by the symbol $\square$.

CHAPTER 1

INTRODUCTION

In this thesis, we will give a detailed mathematical construction of the two-particle Shrödinger operator with point interactions in two dimensions by following the approach described originally in (Dimock and Rajeev, 2004). The formal Hamiltonian operator of this system is given by

$$H = -\frac{\hbar^2}{2m} \sum_{i=1}^{2} \Delta_i - \sum_{1 \leq i,j \leq 2} g\, \delta(\mathbf{x}_i - \mathbf{x}_j) \,, \tag{1.1}$$

where m is the mass of the particles, g is the strength (or coupling constant) of the interaction between the particles and Δ_i is the Laplacian, for i-th particle, and $\hbar = h/(2\pi)$ is the reduced Planck constant. Our two-particle treatment of the system does not assume any symmetry, so particles are assumed to be distinguisable. One can extend the method described here to the Fock space as well but here we only assume that there are two particles without any symmetry.

A single particle interacting only with a Dirac delta potential (that is, one particle version of the above problem) represents quantitatively various physical systems. It is an idealized potential when the de-Broglie wavelength $\lambda = \frac{h}{p}$ of the particle is much larger than the range of the potential, where p is the momentum of the particle. The studies on the applications of the above model and its one-particle version in various dimensions are well-known for a long time in wide range of areas of physics from atomic physics, to molecular physics and nuclear physics (Demkov and Ostrovskii, 1988; Uncu et al., 2005; Cacciapuoti, 2005; Exner and Kovařík, 2015). One of the most famous example for such type of potentials is known as the Kronig-Penney model in solid state physics (Kronig and Penney, 1931; Kittel, 2005). It is essentially based on a Hamiltonian with infinitely many periodic Dirac delta interactions in one dimension, which describes a non-relativistic electron moving in a fixed crystal lattice. This model explains the energy band structure of solids very well and it is exactly solvable. The one dimensional problem with a single Dirac delta potential becomes a standard textbook problem, discussed in various textbooks of Quantum Mechanics (see e.g., (Griffiths and Schroeter, 2018)).

Actually, the model becomes much more interesting if we consider the same Hamiltonian in higher-dimensions. That was first studied by Bethe and Peierls (Bethe and Peierls, 1935) and separately by Thomas (Thomas, 1935) to describe the interaction between proton and neutron in the nucleus by a zero range potential in three dimensions. Bethe and Peierls gave a boundary condition on the wave function which corresponds to delta potential in three dimensions. But it was Thomas who realized the necessity of the renormalization of the coupling constant and he approximated the Hamiltonian by some short range scaled potentials. Then, starting from 1930s, these works stimulated tremendous developments in the field. An extensive historical development and its various applications of the subject with a long list of references is given in the introduction to the monograph (Albeverio et al., 1988).

It is not difficult to see that the above model Hamiltonian in two dimensions is problematic from the physical point of view. This can be immediately seen with a simple scaling argument or by expressing the equation in Fourier space. For simplicity, let us consider only the one particle problem and choose the support of the Dirac delta potential to be at the origin. Then, the time independent Schrödinger equation becomes

$$-\Delta\psi(\mathbf{x}) - g\delta(\mathbf{x})\psi(\mathbf{x}) = E\psi(\mathbf{x}) \ , \qquad (1.2)$$

where we have chosen the units such that $\hbar = 2m = 1$. Under the formal scaling transformation of coordinates by some positive constant, say α, then the left hand side is scaled by a factor $1/\alpha^2$ (using the scaling properties of delta functions and normalization of the bound state wave functions in two dimensions). This implies that we have the same Schrödinger equation except for the rescaled bound state energy by α^2. This means that if you assume that there exists a ground state with some energy, then there should also exist another rescaled ground state energy. Since the scaling parameter is arbitrary, the ground state energy can be lowered arbitrarily, so that the ground state becomes unbounded from below. This is not physically acceptable conclusion. Although the same one dimensional problem is completely well understood physically (see for instance the master thesis (Tunalı, 2014) for some details), its two-dimensional version leads to unphysical results. The problem still exists in higher dimensions although the nature of the problem is somewhat different from its two-dimensional counterpart.

One way to resolve this problem is based on the well known strategy in quantum field theory, namely renormalization. The first step is to smooth out the singularity at short distances by assuming that the form of the potential is only valid down to a scale which we can not access physically. That scale is known as the cut-off. This part of the procedure is known as regularization. Then we have to deduce the physics of the problem in shorter distances by assuming every physical observable remains finite or make senses by fixing some experimentally measured quantity (e.g., bound state energy or phase shift in the scattering process). Then, short distance behavior (or equivalently high energy behavior) can be predicted uniquely, which makes the renormalization procedure remarkable (the magnetic dipole moment of the electron calculated from the renormalization procedure in quantum electrodynamics is confirmed with the experimental result within 14 significant digits). For a pedagogical introduction to renormalization in quantum field theory, see for instance (Kraus and Griffiths, 1992). There are various works on the renormalization of Dirac delta interactions in physics literature from different points of view. In (Gosdzinsky and Tarrach, 1991; Manuel and Tarrach, 1994; Mead and Godines, 1991; Perez and Coutinho, 1991), different regularization schemes are performed in coordinate space or in momentum space (Thorn, 1979; Huang, 1992; Jackiw, 1991; Phillips et al., 1998; Mitra et al., 1998; Henderson and Rajeev, 1998; Nyeo, 2000; Adhikari and Frederico, 1995).

This quantum mechanical problem with Dirac delta potential in two dimensions provides us a way to understand several quantum field theoretical concepts such as regularization, renormalization, dimensional transmutation, quantum anomaly, exact non perturbative solutions to renormalization group equations, etc. Therefore, studying the details of Dirac delta interactions in quantum mechanics may help us to understand better the concepts in the renormalization procedure within a more elementary context. Another important-aspect of point interactions is that they can be exactly solvable, that is, the resolvent can be explicitly calculated in terms of the support and the strength of the Dirac delta potentials (Albeverio et al., 1988).

Actually, from the mathematical point of view, the formal Hamiltonian operator $H = -\Delta - g\delta(\mathbf{x})$ is not even a well defined operator in $L^2(\mathbb{R}^n)$ due to the fact that δ does not map square integrable functions to the square integrable functions. A detailed exposition of the subject (in terms of quadratic forms, nonstandard analysis, and Von

Neumann's approach to self-adjoint extensions of symmetric operators) has been extensively discussed in the monographs (Albeverio and Kurasov, 2000; Albeverio et al., 1988). There is yet another approach to give the above Hamiltonian a well-defined meaning by constructing the resolvent with a suitable limit of the regularized resolvents given in (Rajeev, 1999; Dimock and Rajeev, 2004). This approach can also be applied to some simple field theories (to the bosonic particles interacting through the two-body point interactions in two dimensions) by hoping that these ideas will work in more realistic situations and the cases where standard perturbative approaches do not work, such as in QCD. In this method, the complete information about the spectrum of the system is given by the resolvent formula and the interaction is described by an explicit expression for the resolvent without constructing domains of the operators. The bound state energies are given by the poles of the resolvent and the scattering amplitude is determined by the explicit formula of the resolvent. It has been proved that there exists a densely-defined self-adjoint operator, say H, after the renormalization procedure even if we do not know what the exact formal expression is (Doğan et al., 2012).

Altough there are already several written thesis about the point interactions: (Cacciapuoti, 2005; Altunkaynak, 2005; Gopalakrishnan, 2006; Erman, 2010; Surace, 2010; Tunalı, 2014) summarizing the subject in very detail, we shall here only review the construction of the model, based on the combination of the approximation procedure in the resolvent sense developed in (Dimock and Rajeev, 2004). For the convenience of the physics-oriented reader, we also review the relevant materials from operator theory with given detailed proofs, thus making the thesis self-contained.

The thesis is organised as follows.

In Chapter 2, we shortly introduce the postulates of Quantum Mechanics. Chapter 3 include the basics of operator theory in Hilbert spaces and most of propositions and theorems introduced in this chapter can be found in (Reed and Simon, 1972; Kreyszig, 1978; Hall, 2013; Gustafson and Sigal, 2011; Dimock, 2011). In Chapter 4, we give a brief exposition of the spectrum of operators. Then, we have compiled the Von Neumann's self-adjoint extension theory with some examples from quantum mechanics in Chapter 5. We also finally discuss the bound state problem of the one dimensional Dirac delta potential within the context of self-adjoint extension theory as well as the standard approach given in physics literature. Chapter 6 is the main topic of the thesis, where we study the two dimensional singular two-particle model in quantum mechanics. In this model, we have two particles interacting with each other through Dirac delta potential in two dimensions.

CHAPTER 2

MAIN PRINCIPLES OF QUANTUM MECHANICS

Roughly speaking, quantum mechanics is essentially the physical theory of the microscopic world (e.g., electrons, Hydrogen atom, molecules, etc.). In quantum mechanics, we encounter some peculiar phenomena beyond the limits of our intuition that we are familiar with in daily life (there are some interesting quantum effects, such as the quantum Hall effect, Bose-Einstein condensation, in macroscopic systems as well). In this chapter, we shortly summarize the very basic principles (or postulates) of quantum mechanics. The fact that all the peculiarities appear at very short distances (around $10^{-10}m$) is the main reason why we encounter many confusing results in quantum mechanics (see for instance, discussion on the famous double slit experiment in the first chapter of (Feynman, 1965)). Unfortunately, there is no known formulation of quantum mechanics based on a system of principles directly confirmed by experiments so far. The reason why we are so confident about its validity is based on the fact that all the consequences of the principles are confirmed with experiments (Faddeev and Yakubovskii, 2009).

The list of basic principles is sometimes called axioms but one must be careful about the terminology, it is different from the one used in mathematics literature. Since the laws of quantum mechanics are not complete, the usage of the axioms here does not mean that we can deduce from these "axioms" all other experimental facts in quantum mechanics.

Before giving these list of principles according to the most common formulation of Quantum Mechanics (Copenhagen school), let us first heuristically introduce some notions. In quantum mechanics, we describe the particle moving in $\mathbb{R}^3$ (in this thesis we shall consider the particles moving in $\mathbb{R}^2$ as well) by a complex-valued function (which is also called as *wave function*)

$$\psi(\mathbf{x}, t) \; , \tag{2.1}$$

where $(\mathbf{x}, t) \in \mathbb{R}^3 \times \mathbb{R}$, and $\mathbf{x}$ denotes the position of the particle and t represents the time. The function $\rho_t(\mathbf{x}) = |\psi(\mathbf{x}, t)|^2$ is interpreted as the *probability density* of the particle at

t. According to the probabilistic interpretation, ψ must be normalized

$$\int_{\mathbb{R}^3} |\psi(\mathbf{x}, t)|^2 \, d\mathbf{x} = 1 \,, \tag{2.2}$$

for all $t \in \mathbb{R}$. The position of the particle $\mathbf{x}$ is a quantity which can be measured and is called *observable*. Due to our probabilistic interpretation, it is also a random variable whose *expectation* is defined by

$$E_\psi(\mathbf{x}) = \int_{\mathbb{R}^3} \mathbf{x} |\psi(\mathbf{x}, t)|^2 \, d\mathbf{x} \,. \tag{2.3}$$

In experiments, it is difficult to measure $\mathbf{x}$ directly and we are only able to measure some functions of $\mathbf{x}$. For instance, we can check whether the particle is located inside a certain region Ω of space, say inside a detector (Ω must be Borel set in $\mathbb{R}^3$ to talk about the probability rigorously, see chapter 1 in (Breuer et al., 2002)). The corresponding observable is the characteristic function $\chi_\Omega(\mathbf{x})$ of this set. In particular, the number

$$E_\psi(\chi_\Omega) = \int_{\mathbb{R}^3} \chi_\Omega(\mathbf{x}) |\psi(\mathbf{x}, t)|^2 \, d\mathbf{x} = \int_\Omega |\psi(\mathbf{x}, t)|^2 \, d\mathbf{x} \tag{2.4}$$

gives the probability of finding the particle inside $\Omega \subseteq \mathbb{R}^3$. It is important to notice that, in contrast to classical mechanics, the particle is no longer localized at a certain point in space. In particular, the *mean-square deviation* (or *variance*) $\Delta_\psi(\mathbf{x})^2 = E_\psi(\mathbf{x}^2) - E_\psi(\mathbf{x})^2$ does not vanish in general.

The *phase space* of a quantum system is a complex Hilbert space $\mathcal{H}$ (e.g., we choose $\mathcal{H} = L^2(\mathbb{R}^n)$, see the definition of Hilbert spaces in Chapter 3) and some possible states (pure states in particular) of this system are represented by the elements of this space and denoted by ψ with the unit norm $||\psi|| = 1$.

An observable a corresponds to a linear operator A in this Hilbert space and its expectation, if the system is in the state ψ, is given by the real number

$$E_\psi(A) = \langle \psi, A\psi \rangle = \langle A\psi, \psi \rangle \ , \tag{2.5}$$

where $\langle \cdot, \cdot \rangle$ denotes the inner product in $\mathcal{H}$. Similarly, the mean-square deviation is given by

$$\Delta_\psi(A)^2 = E_\psi(A^2) - E_\psi(A)^2 = ||A - (E_\psi(A))\psi||^2 \ . \tag{2.6}$$

Note that $\Delta_\psi(A) = 0$ if and only if ψ is an eigen state corresponding to the eigenvalue $E_\psi(A)$. In other words,

$$A\psi = E_\psi(A)\psi \ . \tag{2.7}$$

Except for the measurement process, the time evolution of a quantum mechanical system is described in the following way: Given an initial state $\psi(0)$ of the system, there must be a unique vector $\psi(t)$ which represents the state of the system at a later time t (see, for instance, Stone's theorem in (Teschl, 2014)). Then, we will write

$$\psi(t) = U(t)\psi(0) \ . \tag{2.8}$$

Furthermore, we expect that the *superposition of states* must hold from simple consequences of experiments. This implies that $U(t)(\alpha_1\psi_1(0)+\alpha_2\psi_2(0)) = \alpha_1\psi_1(t)+\alpha_2\psi_2(t)$ where $|\alpha_1|^2 + |\alpha_2|^2 = 1$. Hence, $U(t)$ should be linear operator. Moreover, since $\psi(t)$ is a normalized state (i.e., $||\psi(t)|| = 1$), we must have

$$||U(t)\psi|| = ||\psi|| \ . \tag{2.9}$$

Such operators are called *unitary* (see Example 3.33 for exact definition). Next, since we have assumed the uniqueness of solutions to the initial value problem, we must have

$$U(0) = I \ , \tag{2.10}$$

and

$$U(t+s) = U(t)U(s) \ . \tag{2.11}$$

The second condition is just semi-group property. A family of unitary operators $U(t)$ satisfying this property is called a *one-parameter unitary group*. In addition to this, it is natural to assume that this group is strongly continuous, i.e.,

$$\lim_{t \to t_0} U(t)\psi = U(t_0)\psi \ , \tag{2.12}$$

for all $\psi \in \mathcal{H}$. Each such group has an *infinitesimal generator* defined by

$$H\psi := \lim_{t \to t_0} \frac{i}{t}(U(t)\psi - \psi), \tag{2.13}$$

where $D(H) = \{\psi \in \mathcal{H} : \lim_{t \to t_0} \frac{1}{t}(U(t)\psi - \psi) \text{ exists}\}$. This operator must be self-adjoint due to Stone's theorem and it is called the Hamiltonian that corresponds to the energy of the system. If $\psi(0) \in D(H)$, then $\psi(t)$ is a solution of the Schrödinger equation (in suitable units)

$$i\frac{d}{dt}\psi(t) = H\psi(t) \ . \tag{2.14}$$

Solving this equation for a given potential is one of the main problems in quantum mechanics.

In summary, we have the following list of *principles of quantum mechanics*.

1. To every physical system, there is an associated Hilbert space $\mathcal{H}$.The states of the system (according to the pure state theory- simplified idealized case) are described by unit vectors ψ in $\mathcal{H}$. States are in general represented by all positive trace-class linear operators in Hilbert space. In particular, pure states are represented by the projection operator onto the vector ψ. We refer the reader to (Faddeev and Yakubovskii, 2009) for the details.

2. For each observable a, there is an associated linear self-adjoint operator A in $\mathcal{H}$.

3. A pair (ψ, A) determines a probability distribution for the measurement of the observable A in the state ψ and the expectation value for a measurement of a, when the system is in the state ψ is given by $E_\psi(A) = \langle \psi, A\psi \rangle$.

4. The time evolution of the system is given by a strongly continuous one-parameter unitary group

$$U(t) = e^{-\frac{i}{\hbar}Ht} ,$$

where H is the energy observable (generator of the group). This principle is only valid when there is no measurement during the time evolution.

However, one should notice that there is no general prescription for how to find the operator corresponding to a given observable.

The reader interested in the details can consult a mathematically oriented introductory book on quantum mechanics, e.g., see (Faddeev and Yakubovskii, 2009; Schuller, 2016) for the motivation of these principles and all other details. We must also admit that the above list of basic principles or axioms is not complete.

CHAPTER 3

SOME ELEMENTARY NOTIONS AND RESULTS IN OPERATOR THEORY

Before formulating our main problem in this thesis, we would like to first introduce the necessary technical machinery in order to be more clear, pedagogic, and self-contained as much as possible. For this purpose, we shall first discuss some basic notions and some useful theorems in this and the next chapter, starting from the very beginning. Since one must in general deal with unbounded operators in quantum mechanics, we shall start with the discussion of linear operators (not bounded in general) and their properties.

3.1. Linear Operators in Hilbert Spaces

We first shortly recall the most elementary notions in operator theory without going into the details for the sake of being self-contained. As we all know, there are several structures that one can define on sets. One of the most basic structure is known as the metric structure (which is simply the abstract notion of a distance). We refer the reader to (Kreyszig, 1978; Reed and Simon, 1972) for all the details about the concepts introduced in this chapter.

The map $d : M \times M \to \mathbb{R}$ on a set M is called *metric* if it satisfies the following axioms:

1) $d(x, y) \geq 0$,

2) $d(x, y) = 0$ if and only if $x = y$,

3) $d(x, y) = d(y, x)$,

4) $d(x, z) \leq d(x, y) + d(y, z)$ for all $x, y, z \in M$.

If we have metric defined on a set M, then M together with this metric d is called *metric space*.

Then, one can talk about *convergence* of the sequences in the set M in the following way: A sequence of elements $\{x_m\}_{m=1}^{\infty}$ of a metric space M is said to converge to some element x in M if $d(x_m, x) \to 0$ as $m \to \infty$. In this case, we simply write $x_m \to x$ or $\lim_{m\to\infty} x_m = x$. A particular sequence $\{x_m\}_{m=1}^{\infty}$ of a metric space M is called *Cauchy* if for any given $\epsilon > 0$, there exists a positive integer $N \in \mathbb{N}$ such that $n, m \geq N$ implies that $d(x_n, x_m) < \epsilon$ (or we say $d(x_n, x_m) \to 0$ as $n, m \to \infty$). Using the fourth axiom (known as triangle inequality) of the metric, it is easy to show that every convergent sequence is Cauchy (equivalently, if the sequence is not Cauchy, it is not convergent - this is a useful criteria whether a given sequence is convergent or not if you do not have any candidate). Converse statement is in general not correct: Consider a sequence of partial sums $x_N = \sum_{m=0}^{N} 1/m!$ in the set of rationals $\mathbb{Q}$ with the usual metric $d(x, y) = |x - y|$. This partial sum is convergent to the irrational number e, which is not in $\mathbb{Q}$. In a given metric space M, if all the Cauchy sequences in it converge in M, then M is called *complete*.

One can also define the following topological concepts: open, closed sets, and some other derived notions out of them in analogy with the notions that we are familiar with the real numbers. We first define the *open ball* $B(y; r)$ of radius r centered at y as the set $B(y; r) := \{x \in M : d(x, y) < r\}$. A set $O \subset M$ is called *open* if for every $y \in O$, there exists $r > 0$ such that $B(y; r) \subset O$. A point $x \in M$ is called a *accumulation point* (or limit point) of a set $X \subset M$ if there exist a sequence of points $\{x_m\}_{m=1}^{\infty} \in X$ with all $x_m \neq x$ such that $x_m \to x$. Let $X \subset M$, and if X' denotes the set of all the accumulation points of X in M, then the *closure* of X is the set $\overline{X} = X \cup X'$. A set $X \subset M$ is called *closed* if X contains all its accumulation points, that is, $\overline{X} = X$. One can show that $\overline{X}$ is always closed and it is the smallest closed subset containing X. A set X is called *dense* in M if every point of M is an accumulation point of X, or a point of X (or both), that is, $\overline{X} = M$.

A *normed space* is a vector space together with a norm defined on it. The *norm* $||.||$ is a map from the given vector space V to $\mathbb{R}$ satisfying following properties:

1) $||x|| \geq 0$ for all $x \in V$,

2) $||zx|| = |z|\,||x||$ for all $x \in V$ and $z \in \mathbb{C}$,

3) $||x + y|| \leq ||x|| + ||y||$ for all $x, y \in V$,

4) $||x|| = 0$ if and only if $x = 0$.

If the fourth property does not valid, then we have a *semi-norm*. A *Banach space* $\mathcal{B}$ is a complete normed space (complete in the metric defined by the norm $d(x, y) = ||x - y||$).

Definition 3.1 *A Hilbert space $\mathcal{H}$ is a complete inner product space (complete in the metric defined by the inner product: $d(\psi, \varphi) = ||\psi - \varphi|| = \sqrt{\langle \psi - \varphi, \psi - \varphi \rangle}$). Here, the inner product is a map $\langle \cdot, \cdot \rangle : \mathcal{H} \times \mathcal{H} \to \mathbb{C}$ and satisfies the following properties:*

(i) $\langle \varphi, \psi \rangle = \overline{\langle \psi, \varphi \rangle}$ *for all $\varphi, \psi \in \mathcal{H}$. Here the bar denotes the complex conjugation.*

(ii) $\langle \varphi, \psi_1 + z\psi_2 \rangle = \langle \varphi, \psi_1 \rangle + z\langle \varphi, \psi_2 \rangle$ *for all $\varphi, \psi_1, \psi_2 \in \mathcal{H}$ and for all $z \in \mathbb{C}$ (it is linear with respect to the second slot whereas it is anti-linear with respect to the first slot (entry). This is simply a choice commonly used in quantum mechanics literature).*

(iii) $\langle \psi, \psi \rangle \geq 0$ *for all $\psi \in \mathcal{H}$, and $\langle \psi, \psi \rangle = 0$ if and only if $\psi = 0$.*

It follows from the definition that Hilbert spaces are Banach spaces with respect to the norm $||x|| = \sqrt{\langle x, x \rangle}$. Throughout the thesis, we shall deal with operators defined on Hilbert spaces. From now on, we shall denote the vectors in Hilbert spaces by Greek letters simply because of the literature on Quantum Mechanics.

As emphasized in Chapter 2, quantum theory is constructed on the Hilbert spaces, in particular on the set of "square integrable" functions, usually denoted by $L^2(\mathbb{R}^n)$, where n is the dimension of the space on which the particle is moving.

Example 3.1 *Let ψ be a measurable function defined on $\mathbb{R}^n$ with complex values $\mathbb{C}$ (up to equality almost everywhere) and square integrable (in the sense of Lebesgue)*

$$\int_{\mathbb{R}^n} |\psi(\mathbf{x})|^2 \, d\mathbf{x} < \infty \; , \tag{3.1}$$

then, ψ is said to be in $L^2(\mathbb{R}^n)$. The actual meaning of a function in this space is the equivalence class of the function modulo almost everywhere equal (the reason for this is based on the following observation: $||\psi|| = 0$ implies $f \overset{a.e.}{=} 0$, where $a.e.$ stands for almost everywhere). The inner-product in $L^2(\mathbb{R}^n)$ is defined by

$$\langle \varphi, \psi \rangle = \int_{\mathbb{R}^n} \overline{\varphi(\mathbf{x})} \psi(\mathbf{x}) \, d\mathbf{x} \; , \tag{3.2}$$

where $\psi, \varphi \in L^2(\mathbb{R}^n)$. Then $L^2(\mathbb{R}^n)$ is a Hilbert space with the above inner product.

The proof of the completeness of the square integrable function space is rather technical and involves the usage of Lebesgue measure theory (see the Riesz-Fischer theorem given in (Rudin, 1976). Here we stick to the notation $\int\limits_{\mathbb{R}^n} \varphi(\mathbf{x})\ d\mathbf{x}$ for the integrations, altough there are various ones in abstract measure theory (e.g., $d\mu(\mathbf{x})$, or $\mu(d\mathbf{x})$).

One frequently useful fact in the inner product spaces (in particular Hilbert spaces) is the well-known Cauchy-Schwarz inequality

$$|\langle \psi, \varphi \rangle| \leq ||\psi||\,||\varphi||\ , \tag{3.3}$$

for all ψ, φ in $\mathcal{H}$. The idea of the proof is as follows: assume $\varphi, \psi \neq 0$ without loss of generality and then use the decomposition $\psi = c\,\varphi + \chi$ where $\chi \perp \varphi$, and use the positivity of the norms φ and χ.

Corollary 3.2 *If φ_m converges to φ in $\mathcal{H}$, then $\lim\limits_{m\to}\langle \varphi_m - \varphi, \psi\rangle = 0$ for all $\psi \in \mathcal{H}$.*

This is just the result of Cauchy-Schwarz inequality (3.3), i.e., $|\langle \varphi_m - \varphi, \psi \rangle| \leq ||\varphi_m - \varphi||||\psi||$.

Definition 3.3 *The orthogonal complement of the subspace of a Hilbert space $\mathcal{H}$ is defined through the inner product $V^\perp := \{\chi \in \mathcal{H} : \langle \chi, \psi \rangle = 0$ for all $\psi \in V\}$.*

Since we shall use some important results from Hilbert space theory in the subsequent chapters, we are now going to summarize them:

Lemma 3.4 *Let V, W be subspaces of $\mathcal{H}$.*

(i) If $V \subset W$, then $W^\perp \subset V^\perp$.

(ii) $V^\perp$ is a closed linear subspace of $\mathcal{H}$.

(iii) $V \subset (V^\perp)^\perp$.

Proof: (i) Let $\psi \in W^\perp$ and $\varphi \in V$. Then, $\varphi \in W$ (since $V \subset W$), so $\langle \psi, \varphi \rangle = 0$ for all $\varphi \in V$. Then, $\psi \in V^\perp$. (ii) Let $\psi_1, \psi_2 \in V^\perp$, and $z_1, z_2 \in \mathbb{C}$, and $\varphi \in V$. Then, $\langle \varphi, z_1\psi_1 + z_2\psi_2 \rangle = z_1\langle \varphi, \psi_1 \rangle + z_2\langle \varphi, \psi_2 \rangle = 0$, so $z_1\psi_1 + z_2\psi_2 \in V^\perp$. This means that

$V^\perp$ is a linear subspace of $\mathcal{H}$. Let $\{\psi_m\}_{m=1}^{\infty}$ be a sequence in $V^\perp$ converging to $\psi \in \mathcal{H}$. As a simple consequence of the continuity of the inner product, for any $\varphi \in V$ we have $0 = \lim_{m\to\infty} \langle \psi - \psi_m, \varphi \rangle = \langle \psi, \varphi \rangle$ so $\psi \in V^\perp$. (iii) Let $\varphi \in V$. Then, for all $\psi \in V^\perp$, $\langle \varphi, \psi \rangle = \overline{\langle \psi, \varphi \rangle} = 0$, so that $\varphi \in (V^\perp)^\perp$. □

Theorem 3.5 *Let V be a closed subspace (its closure is itself, i.e., $\overline{V} = V$) of a Hilbert space $\mathcal{H}$. Then, for any $\psi \in \mathcal{H}$, there exists a unique $\varphi \in V$ and $\chi \in V^\perp$ such that*

$$\psi = \varphi + \chi \, . \tag{3.4}$$

Moreover, $||\psi||^2 = ||\varphi||^2 + ||\chi||^2$.

The proof of the theorem can be found in (Kreyszig, 1978) and all the details about the counterintuitive infinite dimensional Hilbert spaces (in the sense that many notions, e. g., basis does not have to be exactly the same as the one in finite dimensional vector spaces) can be found in standard textbooks, e.g. (Kreyszig, 1978; Debnath et al., 2005), or even more elementary one (Rynne and Youngson, 2013).

Corollary 3.6 *If V is a closed linear subspace of $\mathcal{H}$, then $V^{\perp\perp} = V$.*

Proof: We have already shown that $V \subset V^{\perp\perp}$ in Lemma 3.4. Suppose that $\psi \in V^{\perp\perp}$. Then, by Theorem 3.5, we can write $\psi = \varphi + \chi$, where $\varphi \in V$ and $\chi \in V^\perp$. Since $\varphi \in V$ and $\psi \in V^{\perp\perp}$, $\langle \psi, \chi \rangle = \langle \varphi, \chi \rangle = 0$. Then, $0 = \langle \psi, \chi \rangle = \langle \varphi + \chi, \chi \rangle = \langle \varphi, \chi \rangle + \langle \chi, \chi \rangle = ||\chi||^2$. This means that $\chi = 0$, or $\psi = \varphi \in V$, which implies $V^{\perp\perp} \subset V$.

Corollary 3.7 *If V is a linear subspace of $\mathcal{H}$, then $V^{\perp\perp} = \overline{V}$.*

Proof: It is clear that $V \subset \overline{V}$, then $\overline{V}^\perp \subset V^\perp$ and $V^{\perp\perp} \subset \overline{V}^{\perp\perp}$ from Lemma 3.4. Since $\overline{V}$ is always closed, $\overline{V}^{\perp\perp} = \overline{V}$ by the Corollary 3.6. Then, $V^{\perp\perp} \subset \overline{V}$. Moreover, by Lemma 3.4, $V \subset V^{\perp\perp}$. Since $V^{\perp\perp}$ is closed and $\overline{V}$ is the smallest closed set containing V, we have $V \subset \overline{V} \subset V^{\perp\perp}$. Therefore, $V^{\perp\perp} = \overline{V}$.

Once we have a new structure in mathematics (here, for instance, Hilbert space), it is natural to study the maps between these structures. Due to the motivation coming from quantum mechanics, we are mainly interested in linear operators on a Hilbert space. For instance, Hamiltonian or Schrödinger operator is one of the most common ones. Many of the results also hold for the ones defined on Banach spaces as well.

Definition 3.8 *A linear operator T is a map $T : D(T) \to \mathcal{H}$, satisfying the linearity*

$$T(\alpha\psi + \beta\varphi) = \alpha T(\psi) + \beta T(\varphi) \; , \tag{3.5}$$

for all ψ, φ in $D(T)$ and for all $\alpha, \beta \in \mathbb{C}$. Here $D(T)$ is called the domain of T (linear subspace of $\mathcal{H}$).

We shall always consider linear operators in this thesis. We will sometimes write the action of the operators as $T(\varphi) = T\varphi$ when it does not lead to confusion throughout the thesis. The linear subspace $Ran(T) := \{T(\varphi) : \varphi \in D(T)\}$ is called the range or the image of the operator T. Moreover, the linear subspace $Ker(T) = \{\varphi \in D(T) : T(\varphi) = 0\}$ is called the kernel of T. This is also called the null space of T.

The notion, namely dense subspace of a metric space can also be extended to the Hilbert spaces, where the metric is induced by the norm $d(\varphi, \psi) = ||\varphi - \psi|| = \sqrt{\langle \varphi - \psi, \varphi - \psi \rangle}$. Let us express the dense subspace definition for Hilbert spaces explicitly:

Definition 3.9 *$D \subseteq \mathcal{H}$ is dense in $\mathcal{H}$ if for any $\psi \in \mathcal{H}$, and for any $\epsilon > 0$, there exists $\varphi \in D$ such that $||\varphi - \psi|| < \epsilon$. Equivalently, for any $\psi \in \mathcal{H}$ there exists a sequence $\{\varphi_n\} \in D$ that converges to ψ. In other words, $\overline{D} = \mathcal{H}$, where $\overline{D}$ denotes the closure of D.*

Example 3.10 *Compactly supported smooth functions $C_0^\infty(\mathbb{R}^n)$ are dense in Schwartz space $S(\mathbb{R}^n)$ (infinitely differentiable "rapidly" decreasing functions) and the Schwartz space $S(\mathbb{R}^n)$ is dense in $L^2(\mathbb{R}^n)$ (see Appendix A for their precise definitions and the proof).*

Definition 3.11 *A linear operator $T : D(T) \to \mathcal{H}$ is said to be densely defined if $D(T)$ is dense in $\mathcal{H}$.*

One of the simplest classes of linear operators is known as the bounded operators due to their simple properties that they satisfy as we shall discuss below.

Definition 3.12 *A linear operator T is said to be bounded if there exists a real number*

$c > 0$ *such that*

$$||T\varphi|| \leq c||\varphi|| \;, \tag{3.6}$$

for all $\varphi \in D(T)$.

The infimum of such c is called the norm of the bounded operator, that is,

$$||T|| := \sup_{\varphi \in \mathcal{D}(\mathcal{T})\setminus\{0\}} \frac{||T\varphi||}{||\varphi||} \;. \tag{3.7}$$

Definition 3.13 *If* $D(T)$ *is dense in* $\mathcal{H}$*, then*

$$||T|| := \sup_{\varphi \in \mathcal{H}\setminus\{0\}} \frac{||T\varphi||}{||\varphi||} \;, \tag{3.8}$$

since if the bounded operator is defined on a dense domain, it can be extended to the whole Hilbert space thanks to the bounded linear extension theorem (BLT), that we shall discuss later on in this chapter.

It is easy to show that the set of bounded operators with $D(T) = \mathcal{H}$ equipped with the pointwise addition and scalar multiplication form a normed space, where the norm of the operator is defined by (3.8). One can further show that this norm space is indeed a Banach space $\mathcal{L}(\mathcal{H})$ (see (Schuller, 2016) for the proof of the completeness of the space). The above definition of norm implies the following useful inequality

$$||T\varphi|| \leq ||T||\, ||\varphi|| \;, \tag{3.9}$$

for all φ and bounded operator T.

The Banach space $\mathcal{L}(\mathcal{H})$ for bounded operators has even an algebraic structure under their compositions (also called product). The composition of bounded operators are also bounded and we have the following useful estimate:

Proposition 3.14 *For any bounded operators* T *and* S*, we have*

$$||TS|| \leq ||T||\, ||S|| \;. \tag{3.10}$$

Proof: Using the definition given in equation (3.8), and the inequality (3.9), the proof is straightforward. □

Let us give some examples for bounded operators:

Example 3.15 *The identity operator I on $\mathcal{H}$ is bounded with norm 1, since $||I\varphi(x)|| = ||\varphi(x)||$.*

A more interesting example for bounded operators is the so-called projection operator:

Example 3.16 *Let P_ψ be the projection operator on the vector ψ in $\mathcal{H}$, defined by*

$$P_\psi \varphi = \langle \psi, \varphi \rangle \psi \ , \tag{3.11}$$

for all $\varphi \in \mathcal{H}$. Using $|P_\psi \varphi| = |\langle \psi, \varphi \rangle| \, ||\psi||$, we find the projection operator is bounded due to the Cauchy-Schwarz inequality (3.3).

Once we have the norm structure on the vector space, we can talk about the continuity of the maps between the vector spaces. In analogy with the definition of continuity, one can define the continuous operator T at the point $\varphi \in \mathcal{H}$ as follows:

$$\varphi_m \underset{m \to \infty}{\to} \varphi \qquad \Longrightarrow \qquad T\varphi_m \underset{m \to \infty}{\to} T\varphi \ . \tag{3.12}$$

Then, we say that T is continuous at φ. This can be put in the following equivalent form, which will be useful when discussing more general class of operators, namely closed operators:

Definition 3.17 *Let T be a linear operator on $\mathcal{H}$ and $\{\varphi_m\}_{m=1}^{\infty}$ be a sequence in $D(T)$ such that $\varphi_m \to \varphi \in \mathcal{H}$ as $m \to \infty$ ($\lim_{m \to \infty} ||\varphi_m - \varphi|| = 0$). If we have*

(i) $T\varphi_m \to \psi \in \mathcal{H}$,

(ii) $T\varphi = \psi$, *where* $\varphi \in D(T)$ *and* $\psi \in Ran(T)$,

then T is called continuous operator at φ.

There is a simple criterion to check whether a given operator is continuous or not, thanks to the following theorem:

Theorem 3.18 *Let T be a linear operator in a Hilbert space $\mathcal{H}$. Then, we have*

(i) T is continuous if and only if T is bounded.

(ii) If T is continuous at a particular element (point) in $\mathcal{H}$, then it is continuous at every point in $\mathcal{H}$.

Proof: We shall give the proof bu using the argument given in (Jordan, 2012).

Proof of the part (a): Suppose that T is a bounded linear operator. We can choose a sequence $\{\varphi_m\}_{m=1}^{\infty}$ converging some limit vector φ. Then,

$$||T\varphi - T\varphi_m|| = ||T(\varphi - \varphi_m)|| \leq ||T||||\varphi - \varphi_m|| \ ,$$

where we have used the linearity of T and the inequality (3.6). Since $||\varphi - \varphi_m|| \to 0$ $m \to \infty$, we deduce from the above inequality that $||T\varphi - T\varphi_m|| \to 0$ as $m \to \infty$. Thus, T is continuous (φ was an arbitrary element in $\mathcal{H}$).

Conversely, we also show that T is bounded if it is continuous. In order to show this, we shall use one of the proof techniques, namely proof by contraposition: Suppose that T is not bounded. This means that for each m there must be a vector ψ_m such that $||T\psi_m|| > m||\psi_m||$. Let $\varphi_m = \frac{1}{m||\psi_m||}\psi_m$. Then, $||\varphi_m|| = \frac{1}{m}$ so $\varphi_m \to 0$ as $m \to \infty$. However, $||T\varphi_m - 0|| > 1$, which means that $T\varphi_m$ can not go to zero as $m \to \infty$. Here we have used $T(0) = 0$ thanks to the linearity. Hence, T is not continuous.

Proof of part (b): Suppose that T is continuous at some point φ_0 in $\mathcal{H}$, that is, for any $\epsilon > 0$ (tolerance number), there exists a $\delta > 0$ such that $||\varphi|| < \delta$ implies that $||T(\varphi_0 + \varphi) - T\varphi_0|| < \epsilon$. By linearity, this implication can be rewritten as $||T(\varphi_0) + T(\varphi) - T(\varphi_0)|| = ||T\varphi|| = ||T(0 + \varphi) - T(0)|| < \epsilon$. Therefore, T is continuous at φ_0 if and only if it is continuous at 0. It follows that if T is continuous at any point, it is continuous everywhere. $\square$

The above theorem simply states that boundedness and continuity are equivalent notions for linear operators. When we lose continuity, we lose boundedness, and vice versa (in contrast to what we have in functions due to the fact that the definition of a bounded function is different from the one given for operators):

$$\text{Bounded Linear Operator} \iff \text{Continuous Linear Operator}$$

In quantum mechanics, the most basic operators, such as the position and the momentum operators, defined on Hilbert spaces are typically unbounded.

Example 3.19 *The position operator X in quantum mechanics is defined as a multiplication operator in $L^2(\mathbb{R})$:*

$$(X\varphi)(x) = x\,\varphi(x)\ ,$$

where its natural domain is given by

$$D(X) = \{\varphi \in L^2(\mathbb{R}) : \int_{\mathbb{R}} |x|^2 |\varphi(x)|^2\, d\mathbf{x} < \infty\}\ .$$

One can show that the domain of this operator is dense in $L^2(\mathbb{R})$ (Hall, 2013) (Although this is not crucial here but it will be important when we discuss adjoint of this operator). For this, we define a subset E_m of $\mathbb{R}$: $E_m := \{x \in \mathbb{R} : |x| < m\}$ so that $\cup_{m=0}^{\infty} E_m = \mathbb{R}$. The characteristic function defined on these subsets are given by

$$\chi_{E_m}(x) = \begin{cases} 1, & x \in E_m, \\ 0, & x \notin E_m\ . \end{cases} \tag{3.13}$$

Then, for any $\psi \in L^2(\mathbb{R})$ we have

$$\int_{\mathbb{R}} |\psi(x)\chi_{E_m}(x)|^2\, dx = \int_{-m}^{m} |\psi(x)|^2\, dx \leq \int_{\mathbb{R}} |\psi(x)|^2\, dx\ , \tag{3.14}$$

and

$$\int_{\mathbb{R}} |(X\psi\chi_{E_m})(x)|^2 \, dx = \int_{\mathbb{R}} |(x\psi(x)\chi_{E_m}(x)|^2 \, dx \tag{3.15}$$

$$\leq \int_{-m}^{m} m^2|\psi(x)|^2 \, dx \tag{3.16}$$

$$\leq m^2 \int_{\mathbb{R}} |\psi(x)|^2 \, dx \; . \tag{3.17}$$

Then, $\psi\chi_{E_m} \in D(X)$. This implies that $D(X)$ is dense in $L^2(\mathbb{R})$ due to the L^2- Lebesgue dominated convergence theorem (Rudin, 1976):

$$\lim_{m\to\infty} \int_{\mathbb{R}} |\psi(x)\chi_m(x) - \psi(x)|^2 \, dx = 0 \; . \tag{3.18}$$

To show that this operator is not bounded, we define an another characteristic function defined on the set $I_m := \{x \in \mathbb{R} : m \leq x \leq m+1\}$

$$\chi_{I_m}(x) := \chi_m(x) = \begin{cases} 1, & x \in I_m, \\ 0, & x \notin I_m \; . \end{cases} \tag{3.19}$$

Then

$$||X\chi_m|| = \left(\int_m^{m+1} |x|^2 \, dx\right)^{1/2} \geq m \left(\int_m^{m+1} 1 \, dx\right)^{1/2} , \tag{3.20}$$

since $x \geq m$ when $x \in [m, m+1]$. Using

$$||\chi_m|| = \left(\int_{\mathbb{R}} |\chi_m(x)|^2 \, dx\right)^{1/2} = \left(\int_m^{m+1} 1 \, dx\right)^{1/2} , \tag{3.21}$$

we find

$$||X\chi_m|| \geq m||\chi_m|| \, . \tag{3.22}$$

Therefore

$$\sup_{\psi \in D(X)\setminus\{0\}} \frac{||X\psi||}{||\psi||} \geq \sup_{\{\chi_m(x)\}_{m=1}^{\infty}} \frac{||X\psi||}{||\psi||} = \sup_{m\geq 1} m = \infty \, . \tag{3.23}$$

Hence, the position operator is not bounded.

Similarly, one can also show that the momentum operator

$$(P\varphi)(x) := -i\hbar \frac{d\varphi}{dx} \, , \tag{3.24}$$

with the following possible choice of the domain $D(P) = S(\mathbb{R})$, which is dense in $L^2(\mathbb{R})$ is not bounded (see the definition of Schwartz space in Appendix A). As we know that Fourier transform is preserving the norms (see Appendix B), it must transform unbounded operators to unbounded operators. Since $S(\mathbb{R})$ is stable under Fourier transform and the derivative operator is just a multiplication operator under Fourier transform, we end up with the result that the momentum operator must be also unbounded as a consequence of the previous example. The above position and momentum operators can actually be extended to $L^2(\mathbb{R}^3)$. Actually, the unboundedness of momentum and position operators are consequence of the algebraic relation, called the canonical commutation relations: $[X, P] := XP - PX = i\hbar$. This can be proved by first noticing that $X^nP - PX^n = i\hbar nX^{n-1} \neq 0$ for all $n \in \mathbb{N}$. Assume that operators are bounded, then taking the norm of the both sides to get $n\hbar < 2||X||\,||P||$, which is a contradiction.

When dealing with unbounded operators, one notion is very useful in order to prove some theorems. This notion can be considered as a generalization of the graph of a function:

Definition 3.20 *The graph of a linear operator T is defined by*

$$\Gamma(T) := \{(\varphi, T\varphi) : \varphi \in D(T)\} \, , \tag{3.25}$$

where $(\cdot,\cdot)$ denotes the pairing. It is a subset of $\mathcal{H} \times \mathcal{H}$, which is again a Hilbert space with inner product defined by:

$$\langle (\varphi_1, \psi_1), (\varphi_2, \psi_2) \rangle = \langle \varphi_1, \varphi_2 \rangle + \langle \psi_1, \psi_2 \rangle \, . \tag{3.26}$$

Definition 3.21 *The operator S is said to be an extension of the operator T if $\Gamma(T) \subseteq \Gamma(S)$. We simply write*

$$T \subseteq S \, . \tag{3.27}$$

Equivalently, $T \subseteq S$ if and only if

(i) $D(T) \subseteq D(S)$,

(ii) $T\varphi = S\varphi$ *for all* $\varphi \in D(T)$.

In other words, S is an extension of the operator T by extending the domain of T to the domain of S and they act in the same way on their common domains. This can also be considered as the definition of the *restriction* of the operator S to the operator T.

Although one should pay attention to the domain of the operators, this is not necessary for bounded operators thanks to the following theorem. This simplifies many technicalities required by the domain issues. There are some cases (e.g., spin systems in quantum mechanics) where you only have bounded operators since the Hilbert space in this case is $\mathbb{C}^n$. In such circumstances, we do not have to deal with domain issues.

Theorem 3.22 (Bounded Linear Transformation (BLT) Theorem) *Any densely defined bounded linear operator*

$$T : D(T) \subseteq \mathcal{H} \to \mathcal{H} \tag{3.28}$$

can be extended uniquely to the whole Hilbert space $\mathcal{H}$.

This theorem basically states the following: We can extend the given linear operator T uniquely by using continuity from its domain $D(T)$ to a linear operator defined on the closure $\overline{D(T)}$ and hence to the operator defined on the whole Hilbert space since T is densely defined. We have to be careful here since this theorem does not state that there can not be unbounded operators which extends T on the whole Hilbert spaces. What it simply says that whenever we have a densely defined bounded linear operator, we can uniquely extend it to the bounded operator defined everywhere in $\mathcal{H}$, which allows you to get rid of dealing with the domain issues. For the sake of simplicity, we leave the proof in Appendix C.

3.2. Closability, Closure, and Closedness

Definition 3.23 *An operator T is called closed if $\Gamma(T)$ is a closed subset of $\mathcal{H} \times \mathcal{H}$.*

Equivalently, the definition of a closed operator can be reexpressed in the following way in order to compare it with continuous (bounded) operators:

Suppose that there exists a sequence of vectors $\{\varphi_m\}_{m=1}^{\infty} \in D(T)$ converging to $\varphi \in \mathcal{H}$ and the sequence of vectors $\{T\varphi_m\}_{m=1}^{\infty}$ converging to $\psi \in \mathcal{H}$. Then, if $\varphi \in D(T)$ and $T\varphi = \psi$, then T is said to be closed. These definitions are equivalent since (φ_m, ψ_m) in $\mathcal{H} \times \mathcal{H}$ converges to (φ, ψ) if and only if φ_n converges to φ in $\mathcal{H}$ and ψ_m converges to ψ in $\mathcal{H}$. It is a simple exercise to show that every bounded operator is closed, but the converse is not always true (Rynne and Youngson, 2013), as the following example shows.

Example 3.24 *The position operator X defined in Example 3.19 is closed. We have already shown that this operator is not bounded. We consider the sequences $\{\varphi_m(x)\}_{m=1}^{\infty}$ and $\{X\varphi_m(x)\}_{m=1}^{\infty}$ such that*

$$\begin{aligned} \varphi_m(x) &\rightarrow \varphi(x) \ , \\ X\varphi_m(x) &\rightarrow \psi(x) \ , \end{aligned}$$

in $L^2(\mathbb{R})$ respectively. Then there exist subsequences (see (Bass, 2013) for its proof)

$$\begin{aligned} \varphi_{m_j}(x) &\stackrel{a.e.}{\rightarrow} \varphi(x) \\ X\varphi_{m_j}(x) = x\varphi_{m_j}(x) &\stackrel{a.e.}{\rightarrow} \psi(x) \ . \end{aligned}$$

We say a sequence of measurable functions $\{\psi_m\}$ converges almost everywhere to ψ and write $\psi_m \stackrel{a.e.}{\rightarrow} \psi$ if there is a set of measure zero such that for x not in this set we have *pointwise convergence $\psi_m(x) \to \psi(x)$. We refer the reader to (Bartle, 2014; Bass, 2013).*

Multiplying first subsequence by x, we get

$$x\varphi_{m_j}(x) \stackrel{a.e.}{\to} x\varphi(x) \ . \tag{3.29}$$

Thus, thanks to the uniqueness of limits (up to measure zero), we must have

$$\underbrace{x\varphi(x)}_{X\varphi(x)} \stackrel{a.e.}{=} \psi(x) \ . \tag{3.30}$$

This equation says that $\varphi(x) \in D(X)$ and $X\varphi(x) = \psi(x)$. This means that the multiplication operator X is closed.

Theorem 3.25 (Closed Graph Theorem) *Let T be linear operator defined on the whole Hilbert space $\mathcal{H}$ into $\mathcal{H}$. Then T is bounded if and only if $\Gamma(T)$ is closed.*

This is actually a particular case of a more general statement, where the operator is defined on Banach spaces. The proof is rather technical so we leave its proof to Appendix C. There are some operators that are not defined on full $\mathcal{H}$ but a dense subspace of $\mathcal{H}$ such that they are not bounded but their graph is closed.

If an operator T is not closed, it seems at first glance that it is always possible to construct its "closure", that is, to extend T to a closed operator $\overline{T}$ by adding to its domain $D(T)$ all vectors $\varphi \in \mathcal{H}$ for which one can find a sequence $\{\varphi_m\}_{m=1}^{\infty} \subseteq D(T)$ such that $\varphi_m \to \varphi$ as $m \to \infty$ and the following limit $\lim\limits_{m\to\infty} T\varphi_m = \psi$ exists. We then naturally set $\overline{T}\varphi = \psi$. However, this procedure does not always work. The expression $\overline{T}\varphi$ may depend on a chosen sequence $\{\varphi_m\}_{m=1}^{\infty}$ converging φ. We say that operator T is closable if this limit exists and its extension is called the closure of T, denoted by $\overline{T}$. In other words, we have the following definition:

Definition 3.26 *An operator T is said to be closable if it has a closed extension. The smallest closed extension of a closable operator T is called closure of T, and it is denoted by $\overline{T}$.*

It is sometimes more convenient to express the above definition in the following way: T

is closable if $\lim_{m\to\infty} \varphi_m = 0$ and $\lim_{m\to\infty} T\varphi_m = \psi \in \mathcal{H}$ for a sequence $\{\varphi_m\}_{m=1}^{\infty} \subset D(T)$ implies that $\psi = 0$. From the above definition, $\psi = \overline{T}0 = 0$. Conversely, suppose that $\varphi \in \mathcal{H}$ such that $\varphi'_m \in D(T) \to \varphi$, $\varphi''_m \in D(T) \to \varphi$, $T\varphi'_m \to \psi'$, and $T\varphi''_m \to \psi''$ as $m \to \infty$. If we define $\varphi_m = \varphi'_m - \varphi''_m$, above definition implies that $\psi' = \psi''$.

It is natural to determine whether a given subspace is a graph of a linear operator or not. The following proposition gives a convenient criteria for this:

Proposition 3.27 *A linear subspace $\Gamma \subseteq \mathcal{H} \times \mathcal{H}$ is the graph of some linear operator T if and only if*

$$(\{0\} \times \mathcal{H}) \cap \Gamma = \{(0,0)\} . \tag{3.31}$$

Proof: Suppose that there exists a linear operator T such that $\Gamma = \Gamma(T)$ and $(0,\psi) \in \Gamma$. Then, $(0,\psi) = (0,T(0)) = (0,0)$. Conversely, suppose that the above condition holds. Then, define the domain of an operator T as $D(T) := \{\varphi : (\varphi,\psi) \in \Gamma \text{ for some } \psi \in \mathcal{H}\}$ and define the action of T on its domain as $T\varphi := \psi$. Then, it is easy to show that T is well-defined (ψ is unique) and linear (see for instance (Hislop and Sigal, 2012)). □

Proposition 3.28 *An operator T is closed if and only if $D(T)$ is complete with respect to the graph norm*

$$||\varphi||^2_{\Gamma(T)} = ||\varphi||^2_{\mathcal{H}} + ||T\varphi||^2_{\mathcal{H}} , \tag{3.32}$$

which is induced by the inner product

$$\langle \varphi_1, \varphi_2 \rangle_{\Gamma(T)} = \langle \varphi_1, \varphi_2 \rangle_{\mathcal{H}} + \langle T\varphi_1, T\varphi_2 \rangle_{\mathcal{H}} .$$

Proof: Suppose T is closed and let $\{\varphi_m\}_{m=1}^{\infty}$ be a Cauchy sequence in $D(T)$ with respect to the graph norm which is defined by Equation (3.32). Using Equation (3.32), we get

$$||\varphi_n - \varphi_m||^2_{\Gamma(T)} = ||\varphi_n - \varphi_m||^2_{\mathcal{H}} + ||T\varphi_n - T\varphi_m||^2_{\mathcal{H}} . \tag{3.33}$$

Since the left hand side of the Equation (3.33) vanishes as $n,m \to \infty$, we must have $||\varphi_n - \varphi_m||_{\mathcal{H}} \to 0$ and $||T\varphi_n - T\varphi_m||_{\mathcal{H}} \to 0$ as $n,m \to \infty$. That is the sequences $\{\varphi_m\}_{m=1}^{\infty}$ and $\{T\varphi_m\}_{m=1}^{\infty}$ are Cauchy in $\mathcal{H}$. So, they must be convergent (since Hilbert space is compete inner product space). Say the limits of these sequences are φ and ψ.

This means $||\varphi_m - \varphi||_{\mathcal{H}} \to 0$ and $||T\varphi_m - \psi||_{\mathcal{H}} \to 0$. Since T is assumed to be closed, $\varphi \in D(T)$ and $\psi = T\varphi \in Ran(T)$. Using these convergences and the definition of $||\cdot||_{\Gamma(T)}$, we see that the Cauchy sequence $\{\varphi_m\}_{m=1}^{\infty}$ converges to $\varphi \in D(T)$ with respect to the $||\cdot||_{\Gamma(T)}$. That is $D(T)$ is compete with respect to the graph norm.

Conversely, suppose $D(T)$ is complete with respect to the graph norm. Also assume the sequence $\{(\varphi_m, T\varphi_m)\}_{m=1}^{\infty}$ converges to $(\varphi, \psi) \in \mathcal{H} \times \mathcal{H}$, that is $||\varphi_m - \varphi||_{\mathcal{H}} \to 0$ and $||T\varphi_m - \psi||_{\mathcal{H}} \to 0$. Since they are convergent, they must be Cauchy with respect to the $||\cdot||_{\mathcal{H}}$. Using this fact and the definition of graph norm, we see that the sequence $\{\varphi_m\}_{m=1}^{\infty}$ is Cauchy with respect to the $||\cdot||_{\Gamma(T)}$. Since $D(T)$ is complete with respect to the graph norm, there exists a function $\phi \in D(A)$ such that $||\varphi_m - \phi||_{\Gamma(T)} \to 0$ as $m \to \infty$. This implies that $||\varphi_m - \phi||_{\mathcal{H}} \to 0$ and $||T\varphi_m - T\phi||_{\mathcal{H}} \to 0$. By the uniqueness of limit $\varphi = \phi \in D(T)$ and $\psi = T\phi = T\varphi$. That is $(\varphi, \psi) \in \Gamma(T)$. Hence T is closed (see for instance (Berezansky et al., 1996)). □

If we try to obtain a closed extension of an operator, we simply take the closure of its graph. But, in general, the closure of the graph of the operator may not be a graph of an operator (see (Reed and Simon, 1972) chapter viii problem 1). The following theorem gives the condition for this problem.

Proposition 3.29 *If T is closable, then $\Gamma(\overline{T}) = \overline{\Gamma(T)}$.*

Proof: First of all, our aim is to show $\overline{\Gamma(T)}$ is a graph of some linear operator if we assume that T is closable. For this purpose, suppose T is closable, then there exists a closed operator S such that $\Gamma(T) \subseteq \Gamma(S)$. Then, $\overline{\Gamma(T)} \subseteq \Gamma(S)$. If $(0, \psi) \in \overline{\Gamma(T)} \subseteq \Gamma(S)$ for any $\psi \in \mathcal{H}$, we must have $\psi = 0$ by Proposition 3.27 (since $\Gamma(S)$ is the graph of a linear operator). Hence $\overline{\Gamma(T)}$ is a graph of a linear operator by Proposition 3.27. Thanks to the definition of closure of a space, $\overline{\Gamma(T)}$ is the smallest closed space containing $\Gamma(T)$, then $\Gamma(T) \subseteq \overline{\Gamma(T)} \subseteq \Gamma(\overline{T})$. On the other hand, $\overline{T}$ is the smallest closed extension of T, that is $\Gamma(T) \subseteq \Gamma(\overline{T}) \subseteq \overline{\Gamma(T)}$. Hence, $\Gamma(\overline{T}) = \overline{\Gamma(T)}$ (see for instance (Reed and Simon, 1972)). □

Proposition 3.30 *An operator T is closed if and only if*

$$T = \overline{T}\ . \tag{3.34}$$

Proof: Suppose T is closed, then its graph $\Gamma(T)$ is closed, that is $\overline{\Gamma(T)} = \Gamma(T)$. On the other hand, since T is assumed to be closed then it must be closable. Therefore, from Proposition 3.29 we also have $\Gamma(\overline{T}) = \overline{\Gamma(T)}$. Combining all these, we obtain $\Gamma(T) = \Gamma(\overline{T})$, implying that $T = \overline{T}$.

Conversely if $\overline{T} = T$, then

$$\Gamma(T) = \Gamma(\overline{T}) = \overline{\Gamma(T)} \ . \tag{3.35}$$

Hence, $\Gamma(T)$ is closed, or equivalently T is a closed operator (see for instance (Reed and Simon, 1972)). □

Apart from the closed and bounded operators, the most important classes of operators in Quantum Mechanics are known as symmetric and self-adjoint operators, as we shall define them in the next section.

3.3. Symmetric and Self-Adjoint Operators

Definition 3.31 *Let $T : D(T) \to \mathcal{H}$ be a densely defined linear operator on $\mathcal{H}$. The adjoint of the operator T is defined by*

$$D(T^*) := \{\psi \in \mathcal{H} : \exists \eta \in \mathcal{H} \text{ such that } \langle \psi, T\varphi \rangle = \langle \eta, \varphi \rangle \text{ for all } \varphi \in D(T)\} \ , \tag{3.36}$$

and its action on its domain is defined by

$$T^* \psi := \eta \ . \tag{3.37}$$

Roughly speaking, the above definition of the adjoint operator corresponds to a flipping operation of the initial operator T in the inner product to the other slot (entry) of the inner product:

$$\langle \psi, T\varphi \rangle = \langle T^* \psi, \varphi \rangle \ . \tag{3.38}$$

However, one must be careful about this formal operation since we have to be sure that the adjoint of the operator should act on the elements of its domain on the right hand side. That is why we first define the domain of the adjoint operator and then the action of it on its domain. *The notation for the adjoint of an operator in physics literature is usually denoted by* $T^\dagger$. One may recall that the adjoint of an operator in $\mathbb{C}^n$ are given by $(T^*)_{ij} = \overline{T}_{ji}$, where $i, j = 1, \dots, n$.

If we go back to the definition of the adjoint operator, we have to be sure that η must be unique. Otherwise, the adjoint is not well-defined, that is, the action of adjoint on its domain gives different results.

Proposition 3.32 *T^* is well-defined.*

Proof: Suppose that there are two vectors η and η' satisfying $\langle \psi, T\varphi \rangle = \langle \eta, \varphi \rangle$, and $\langle \psi, T\varphi \rangle = \langle \eta', \varphi \rangle$ for any $\varphi \in D(T)$. Subtracting these equations from each other, we get

$$\langle \eta - \eta', \varphi \rangle = 0 \ , \tag{3.39}$$

for any $\varphi \in D(T)$. Since $D(T)$ is dense in $\mathcal{H}$, Equation (3.39) implies that $\eta - \eta' = 0$, i.e., $\eta = \eta'$ that is what we wanted to show (Since $D(T)$ is dense in $\mathcal{H}$, there exists a sequence $\{\varphi_m\}_{m=1}^{\infty} \in D(T)$ converging to $\eta - \eta' \in \mathcal{H}$. Thanks to the continuity of inner product we have $0 = \lim_{m\to\infty} \langle \eta - \eta', \varphi_m \rangle = \langle \eta - \eta', \lim_{m\to\infty} \varphi_m \rangle = \langle \eta - \eta', \eta - \eta' \rangle$) (see for instance (Schuller, 2016)). □

Example 3.33 *An operator U on a Hilbert space $\mathcal{H}$ is said to be unitary if U is surjective (onto) and preserves inner products, i.e., $\langle U\psi, U\varphi \rangle = \langle \psi, \varphi \rangle$ for all $\psi, \varphi \in \mathcal{H}$. It follows from the definition that U preserves norm as well: $||U\psi|| = ||\psi||$ for all $\psi \in \mathcal{H}$. Hence it is bounded and $||U|| = 1$. Using $\langle \psi, \varphi \rangle = \langle U\psi, U\varphi \rangle = \langle U^*U\psi, \varphi \rangle$, so we have $\langle (U^*U - I)\psi, \varphi \rangle = 0$ for all $\varphi, \psi \in \mathcal{H}$. Then, choosing $\varphi = (U^*U - I)\psi$, we obtain $U^*U = I$. Hence, $U(U^*U)\psi = U\psi$ or $(UU^*)\chi = \chi$, where $\chi = U\psi \in \mathcal{H}$, where we have used the fact that the range of U is the full Hilbert space.*

Definition 3.34 *A densely defined operator $T : D(T) \to \mathcal{H}$ is called symmetric (or Hermitian) if*

$$\langle \psi, T\varphi \rangle = \langle T\psi, \varphi \rangle \ , \tag{3.40}$$

for all $\psi, \varphi \in D(T)$.

Definition 3.35 *A densely defined operator $T : D(T) \to \mathcal{H}$ is self-adjoint if $T = T^*$. This means that*

(i) $D(T) = D(T^*)$ *and*

(ii) $T\varphi = T^*\varphi$ *for any* $\varphi \in D(T)$.

Every self-adjoint operator is symmetric, but in the unbounded case, the converse is in general not true. The domain of the operator and the domain of its adjoint may not be the same.

Definition 3.36 *A symmetric operator T is called essentially self-adjoint if its closure $\overline{T}$ is self-adjoint.*

Since it is not so easy to find explicitly the adjoint domain of a given operator, it is hard to check whether an operator is self-adjoint or not. For this reason, there are some useful criteria to determine whether the operator is self-adjoint as we shall see later on.

The following theorem is one of the main reasons why we have to deal with so many technical domain issues in quantum mechanics and in this thesis in particular. The reason for that lies in the fact that most important operators in quantum theory (like position and momentum as we have seen) are unbounded operators but they have to obey the symmetry condition in some sense. The theorem below states that this can not happen, i.e., the unbounded operators in quantum mechanics can not be everywhere defined, so they have to be defined on a dense subspace of Hilbert spaces, namely on their domains, where all the trivial algebraic operations (addition, composition) must be carefully performed since $T + S$ may not be defined when $D(T) \cap D(S) = \varnothing$.

Theorem 3.37 (The Hellinger-Toeplitz Theorem) *Let T be a symmetric operator defined on the whole $\mathcal{H}$. Then T is bounded.*

Proof: Let $\{(\varphi_m, T\varphi_m)\}_{m=1}^{\infty}$ be sequence in $\Gamma(T)$ such that

$$\lim_{m\to\infty} (\varphi_m, T\varphi_m) = (\varphi, \psi) \in \mathcal{H} \times \mathcal{H} \ . \tag{3.41}$$

Our aim is to show $(\varphi, \psi) \in \Gamma(T)$, i.e., $\psi = T\varphi$. Let ϕ be a nonzero element in $D(T) = \mathcal{H}$. Using continuity of inner product and symmetry of T, we get $\langle \phi, \psi \rangle =$

$\langle \phi, \lim_{m\to\infty} T\varphi_m \rangle = \lim_{m\to\infty} \langle \phi, T\varphi_m \rangle = \lim_{m\to\infty} \langle T\phi, \varphi_m \rangle = \langle T\phi, \lim_{m\to\infty} \varphi_m \rangle = \langle T\phi, \varphi \rangle = \langle \phi, T\varphi \rangle$. So, $\langle \phi, \psi - T\varphi \rangle = 0$, which leads $\psi = T\varphi$. Hence $\Gamma(T)$ is closed (see for instance (Reed and Simon, 1975)). □

Actually, the above theorem is direct corollary of the closed graph theorem 3.25. For symmetric operators, we have a very useful result to estimate symmetric operators that we are going to use later on.

Proposition 3.38 *Suppose T is a symmetric operator on a Hilbert space $\mathcal{H}$ and $z = \lambda + i\mu \in \mathbb{C}$ where $\lambda, \mu \in \mathbb{R}$. Then,*

$$||(T - zI)\varphi||^2 = ||(T - \lambda I)\varphi||^2 + ||\mu\varphi||^2 \; . \tag{3.42}$$

Proof: Using the fact that T is symmetric, we have

$$\begin{aligned} ||(T - zI)\varphi||^2 &= \langle (T - zI)\varphi, (T - zI)\varphi \rangle \\ &= ||(T - \lambda I)\varphi||^2 + \langle T\varphi, -i\mu I\varphi \rangle + \langle -\lambda I\varphi, -i\mu I\varphi \rangle \\ &+ \langle -i\mu I\varphi, T\varphi \rangle + \langle -i\mu I\varphi, -\lambda I\varphi \rangle + ||\mu\varphi||^2 \\ &= ||(T - zI)\varphi||^2 = ||(T - \lambda I)\varphi||^2 + ||\mu\varphi||^2 \; , \end{aligned}$$

for any $\varphi \in D(T)$. □

Proposition 3.39 *Let T and S be linear densely defined operators on $\mathcal{H}$.*

(i) If $T \subseteq S$, then $S^* \subseteq T^*$.

(ii) If T is symmetric, then $T \subseteq T^*$.

(iii) If T is symmetric, then $T^{**} \subseteq T^*$.

Proof: (i) Let us first show that $D(S^*) \subseteq D(T^*)$: Suppose that $\psi \in D(S^*)$, then from the definition of S^* there exists a unique $\eta \in \mathcal{H}$ such that $\langle \psi, S\phi \rangle = \langle \eta, \phi \rangle$ for all $\phi \in D(S)$. Since we are given $T \subseteq S$, we get

$$\langle \psi, T\varphi \rangle = \langle \psi, S\varphi \rangle = \langle \eta, \varphi \rangle \; , \tag{3.43}$$

for all $\varphi \in D(T) \subseteq D(S)$, that is $\psi \in D(T^*)$, implying that $D(S^*) \subseteq D(T^*)$. What is left is to show that $T^*\psi = S^*\psi$ for all $\psi \in D(S^*)$. From the Equation (3.43) we have

$$S^*\psi = \eta = T^*\psi \ , \tag{3.44}$$

for all $\psi \in D(S^*)$.

(ii) First, we need to show that $D(T) \subseteq D(T^*)$. Let $\psi \in D(T)$ and define $\eta := T\psi$. Since T is symmetric

$$\langle \psi, T\varphi \rangle = \langle T\psi, \varphi \rangle = \langle \eta, \varphi \rangle \ , \tag{3.45}$$

for any $\varphi \in D(T)$. Then $\psi \in D(T^*)$, so $D(T) \subseteq D(T^*)$. From above we have $T^*\psi := \eta = T\psi$ for all $\psi \in D(T)$, which completes the proof of (ii).

(iii) If T is symmetric, then $T \subseteq T^*$ by (ii). This implies $D(T) \subseteq D(T^*)$ or $\overline{D(T)} \subseteq \overline{D(T^*)}$. On the other hand, thanks to the definition of symmetric operators, domain of T must be dense in $\mathcal{H}$, i.e., $\overline{D(T)} = \mathcal{H}$. Therefore we have $\mathcal{H} = \overline{D(T)} \subseteq \overline{D(T^*)} \subseteq \mathcal{H}$. Thus $\overline{D(T^*)} = \mathcal{H}$ (adjoint of a symmetric operator is densely defined). Then the result $T^{**} \subseteq T^*$ immediately follows from (i) (see for instance (Schuller, 2016)). □

Lemma 3.40 *The self-adjoint extension of a self-adjoint operator must coincide with itself.*

Proof: Suppose T is a self-adjoint operator and $T \subseteq S$ where S is self-adjoint, then

$$T \subseteq S = S^* \underset{\text{Proposition 3.39}}{\subseteq} T^* = T, \text{ then } S = T. \tag{3.46}$$

See for instance (Schuller, 2016). □

In more technical words, we simply say that a self-adjoint operator is maximal with respect to self-adjoint extension. In fact, self-adjoint operators are maximal even with respect to symmetric extension. If S was just symmetric operator, then we would have $S \subseteq S^*$ instead of $S = S^*$ in the Equation (3.46) thanks to Proposition 3.39.

In the following chapters we shall use the following nice property of symmetric operators:

Proposition 3.41 *Let T be a densely defined linear operator on $\mathcal{H}$. Then,*

$$Ker(T^*) = Ran(T)^{\perp} \ . \tag{3.47}$$

Proof: $(\subseteq)$: for any $\psi \in Ker(T^*)$, $T^*\psi = 0$, and using the definition of T^* we have

$$0 = \langle T^*\psi, \varphi \rangle = \langle \psi, T\varphi \rangle \ , \tag{3.48}$$

for all $\varphi \in D(T)$. In other words, $\psi \in Ran(T)^{\perp}$, therefore $Ker(T^*) \subseteq Ran(T)^{\perp}$.

$(\supseteq)$: for any $\psi \in Ran(T)^{\perp}$, using definition of T^* we get

$$0 = \langle \psi, T\varphi \rangle = \langle T^*\psi, \varphi \rangle \ , \tag{3.49}$$

for any $\varphi \in D(T)$. On the other hand, since $D(T)$ is dense in $\mathcal{H}$, we have $T^*\psi = 0$, i.e., $\psi \in Ker(T^*)$. Therefore $Ker(T^*) \supseteq Ran(T)^{\perp}$ Hence $Ker(T^*) = Ran(T)^{\perp}$ (see for instance (Schuller, 2016)). □

Corollary 3.42 *If T is densely defined linear operator on $\mathcal{H}$, then*

$$\mathcal{H} = Ker(T^*) \oplus \overline{Ran(T)} \ . \tag{3.50}$$

Proof: Since $Ker(T^*)$ is written as the orthogonal complement of $Ran(T)$, it is closed by Lemma 3.4. Then, it follows from Theorem 3.5 Hilbert space $\mathcal{H}$ can be decomposed as $\mathcal{H} = Ker(T^*) \oplus Ker(T^*)^{\perp} = Ker(T^*) \oplus Ran(T)^{\perp\perp}$. Thanks to the Corollary 3.7, we obtain the desired result. □

Another key notion of operators is their inverse and it will be particularly important in the study of the spectrum of the operators that we are going to discuss in the next chapter.

3.4. Inverse and Invertibility

Definition 3.43 *Suppose T is a linear operator on $\mathcal{H}$. An operator S is called the inverse of T if $D(S) = Ran(T)$, $D(T) = Ran(S)$ (in order to have a well defined composition of the operators), and*

$$ST = I_{Ran(S)} , \tag{3.51}$$

$$TS = I_{Ran(T)} . \tag{3.52}$$

The inverse of T is denoted by T^{-1}.

It is not difficult to show from the above definition that the inverse must be unique if it exists. Finding the inverse of an operator T is equivalent to solving the following inhomogenous equation

$$T\psi = \chi , \tag{3.53}$$

for all χ in $Ran(T)$. This will be useful for our purposes when we are looking for the inverse of a particular operator associated with our main problem in Chapter 6. If you need to check whether a given operator T has an inverse, the best criterion is:

An operator T has an inverse if and only if

$$Ker(T) = \{0\} . \tag{3.54}$$

The basic idea of the proof is as follows: Suppose $\varphi_1, \varphi_2 \in D(T)$ and $T\varphi_1 = \psi = T\varphi_2$. Then, $0 = T\varphi_1 - T\varphi_2 = T(\varphi_1 - \varphi_2)$ from linearity. This means that $\varphi_1 - \varphi_2 \in Ker(T) = \{0\}$, implying $\varphi_1 = \varphi_2$. This allows us to define an operator $T^{-1} : Ran(T) \to D(T)$ with $T^{-1}\psi = \varphi$, where $T\varphi = \psi$. The operator T^{-1} is well-defined and linear. Furthermore, $\varphi = T^{-1}\psi = T^{-1}(T\varphi)$, i.e., $T^{-1}T = I_{D(T)}$, and $TT^{-1}\psi = T\varphi = \psi$ for $\psi \in Ran(T)$, i.e., $TT^{-1} = I_{Ran(T)}$. Conversely, suppose that T^{-1} exists. If $\varphi \in Ker(T)$, then $\varphi = T^{-1}T\varphi = 0$, so $Ker(T) = \{0\}$ (see for instance (Hislop and Sigal, 2012)).

Lemma 3.44 *If T is a symmetric operator on $\mathcal{H}$ and its inverse exists, then T^{-1} is also symmetric.*

Proof: Since $\langle \psi, T\varphi \rangle = \langle T\psi, \varphi \rangle$ for all $\varphi, \psi \in D(T)$, and let $T\psi = \chi$ and $T\varphi = \xi$, we have $\langle T^{-1}\chi, \xi \rangle = \langle \chi, T^{-1}\xi \rangle$ for all $\chi, \xi \in D(T^{-1})$. □

Definition 3.45 *A linear operator T is called invertible if its inverse is bounded on the entire Hilbert space $\mathcal{H}$ (or it has a bounded inverse everywhere).*

As a consequence of the Proposition 3.22 (BLT theorem), an invertible operator T must also be onto in addition to being one-to-one since

$$Ran(T) = D(T^{-1}) = \mathcal{H} \ . \tag{3.55}$$

The conditions $Ker(T) = \{0\}$ and $Ran(T) = \mathcal{H}$ are necessary conditions for T to be invertible.

Proposition 3.46 *Let T and S be two linear operators. If T and S are invertible and S is bounded, then the composition operator ST is defined on $D(ST) = D(T)$ and invertible and $(ST)^{-1} = T^{-1}S^{-1}$.*

Proof: Since S is bounded, its domain can be extended to the entire Hilbert space $\mathcal{H}$ so that $D(ST) = D(T) \cap D(S) = D(T)$. From the definition of compositions, we must have $D(S) = Ran(T) = D(T^{-1})$ and $D(S)$ is entire Hilbert space, consistent with the invertibility of T.

Let T and S be invertible operators, then there exists inverse operators T^{-1} and S^{-1} which are bounded. Clearly we have $STT^{-1}S^{-1} = I$, and $T^{-1}S^{-1}ST = I$, where I is the identity operator on $\mathcal{H}$. This means that ST has an inverse and given by $T^{-1}S^{-1}$. Using the assumption that S and T are invertible, we have

$$||T^{-1}S^{-1}|| \leq ||S^{-1}|| \, ||T^{-1}|| < \infty \ , \tag{3.56}$$

by Proposition 3.14 (see for instance (Gustafson and Sigal, 2011)). □

Proposition 3.47 *Suppose that T is a bounded operator from $\mathcal{H}$ to $\mathcal{H}$ and satisfies $||T|| < 1$. Then the operator $I - T$ is invertible, with the inverse given by the following convergent* *series (Neumann series)*

$$(I - T)^{-1} = I + T + T^2 + T^3 + \cdots \ . \tag{3.57}$$

Proof: Since $||T|| < 1$, the geometric series $\sum_{m=0}^{\infty} ||T||^m$ converges in $\mathbb{R}$. By Proposition 3.14, we have $||T^m|| \leq ||T||^m$ for any $m \in \mathbb{N}_0$, so that $\sum_{m=0}^{\infty} ||T^m||$ converges in $\mathbb{R}$ by comparison test. Therefore, the series $\sum_{m=1}^{\infty} T^m$ converges in Banach space $\mathcal{L}(\mathcal{H})$ - set of bounded operators form a complete normed vector space - (Let $\epsilon > 0$ and define the Nth partial sum $S_k := \sum_{m=0}^{k} T^m$. Since $\sum_{m=0}^{\infty} ||T^m||$ converges, the partial sums $\sum_{m=0}^{k} ||T^m||$ form a Cauchy sequence, i.e., there exists $N \in \mathbb{N}$ such that $\sum_{m=0}^{k} ||T^m|| - \sum_{m=0}^{l} ||T^m|| = \sum_{m=l+1}^{k} ||T^m|| < \epsilon$ whenever $k, l \geq N$. Hence, by the triangle inequality we get $||S_k - S_l|| \leq \sum_{m=l+1}^{k} ||T^m|| < \epsilon$ when $k, l \geq N$. This simply says that $\{S_k\}$ form a Cauchy sequence so it converges since $\mathcal{L}(\mathcal{H})$ is complete. Thus, $\sum_{m=1}^{\infty} T^m$ converges in Banach space $\mathcal{L}(\mathcal{H})$). Let us now find the limit. It is easy to realize that

$$\begin{aligned} ||(1-T)S_k - 1|| &= ||S_k - TS_k - 1|| = ||\sum_{m=0}^{k} T^m - \sum_{m=0}^{k} T^{m+1} - 1|| && (3.58)\\ &= ||-T^{k+1}|| && (3.59)\\ &\leq ||T||^{k+1} \ . && (3.60) \end{aligned}$$

Thanks to $||T|| < 1$, we immediately conclude that $\lim_{k\to\infty} (1-T)S_k = 1$ in $\mathcal{L}(\mathcal{H})$. If $S_k \to S$ in $\mathcal{L}(\mathcal{H})$, then $(1-T)S_k \to (1-T)S$ in $\mathcal{L}(\mathcal{H})$ by $||(1-T)S_k - (1-T)S|| = ||(1-T)(S_k - S)|| \leq ||(1-T)|| \, ||S_k - S||$. Hence, we obtain $(1-T)S = (1-T)\lim_{k\to\infty} S_k = \lim_{k\to\infty} (1-T)S_k = 1$.

$$(I - T)^{-1} = \sum_{m=0}^{\infty} T^m \ . \tag{3.61}$$

See for instance (Hall, 2013) □

Theorem 3.48 *Let T be an invertible linear operator and S be bounded and satisfies $||ST^{-1}|| < 1$. Then the operator $T + S$ is invertible with domain $D(T + S) = D(T)$.*

Proof: Existence of T^{-1} implies the following relation $T + S = (I + ST^{-1})T$. Invertibility of T and the consequence of Proposition 3.47 suggest that $T + S$ must have an inverse and its inverse is bounded

$$||(T+S)^{-1}|| = ||T^{-1}(I+ST^{-1})^{-1}|| \leq ||T^{-1}|| \, ||(I+ST^{-1})^{-1}|| \,, \tag{3.62}$$

where we have used Proposition 3.14. Hence $T + S$ is invertible (see (Gustafson and Sigal, 2011)). □

3.5. Some Useful Relations Among the Combined Notions of Linear Operators

We have a very powerful theorem about the closability and the adjoint of an operator, from which we draw several useful conclusions.

Theorem 3.49 *Let T be a densely defined linear operator on a Hilbert space $\mathcal{H}$. Then we have*

(i) T^* is closed.

(ii) T is closable if and only if $D(T^*)$ is dense, in which case $T^{**} = \overline{T}$.

(iii) If T is closable, then $(\overline{T})^* = T^*$.

Before proving the theorem we shall define some unitary operators, which simplify the proofs a lot. Let us define two unitary operators on $\mathcal{H} \times \mathcal{H}$:

$$U(\varphi, \psi) := (\psi, \varphi) \,, \tag{3.63}$$

$$V(\varphi, \psi) := (-\psi, \varphi) \,, \tag{3.64}$$

where $\varphi, \psi \in \mathcal{H}$. From the above definitions, we have

$$U^{-1}(\varphi, \psi) = (\psi, \varphi)$$

and

$$V^{-1}(\varphi, \psi) = (\psi, -\varphi) \ .$$

Moreover,

$$U^{-1}V(\varphi, \psi) = U^{-1}(-\psi, \varphi) = (\varphi, -\psi) = V^{-1}(\psi, \varphi) = V^{-1}U(\varphi, \psi), \qquad (3.65)$$

or

$$U^{-1}V = V^{-1}U \ . \qquad (3.66)$$

Suppose that T^{-1} exists. Then, for any $\varphi \in D(T)$ and $\psi = T\varphi$, we have $U(\varphi, T\varphi) = (T\varphi, \varphi) = (\psi, T^{-1}\varphi) \in \Gamma(T^{-1})$, and vice versa for the reverse inclusion. Hence,

$$U(\Gamma(T)) = \Gamma(T^{-1}) \ . \qquad (3.67)$$

This is very similar to the rule for the graphs of inverse functions in Calculus, namely, the graph of the inverse of a function f^{-1} is obtained by reflecting the graph of f about the line $y = x$.

Proposition 3.50 *For any unitary map V and any subspace M of Hilbert space, we have*

$$(VM)^{\perp} = V(M^{\perp}) \ . \qquad (3.68)$$

Proof: $(VM)^{\perp} \subseteq V(M^{\perp})$: Let $\psi \in (VM)^{\perp}$. Then, $0 = \langle \psi, V\varphi \rangle = \langle V^{*}\psi, \varphi \rangle = \langle V^{-1}\psi, \varphi \rangle$, where $\varphi \in M$. This implies that $V^{-1}\psi \in M^{\perp}$. Then we have $V^{-1}\psi = \phi$ for some $\phi \in M^{\perp}$. Then, $\psi = V\phi$ which implies that $\psi \in V(M^{\perp})$. Therefore $(VM)^{\perp} \subseteq V(M^{\perp})$.

$V(M^{\perp}) \subseteq (VM)^{\perp}$: Conversely, let $\psi \in V(M^{\perp})$. Then, $\psi = V\phi$ for some $\phi \in M^{\perp}$ and $0 = \langle \phi, \chi \rangle = \langle V^{-1}\psi, \chi \rangle = \langle V^{*}\psi, \chi \rangle = \langle \psi, V\chi \rangle$ for any $\chi \in M$. This means that $\psi \in (VM)^{\perp}$. Hence we get $V(M^{\perp}) \subseteq (VM)^{\perp}$ which completes our proof. $\square$

Proposition 3.51 *Let V be the unitary operator defined in equation (3.64). For any* *densely defined linear operator T from $\mathcal{H}$ to $\mathcal{H}$, we have*

$$\Gamma(T^*) = V(\Gamma(T))^\perp = V(\Gamma(T)^\perp) \ . \tag{3.69}$$

Proof: Suppose $\varphi \in D(T)$ and $\psi \in D(T^*)$. Using the definition of the unitary operator V and inner product on $\mathcal{H} \times \mathcal{H}$, we have

$$\langle V(\varphi, T\varphi), (\psi, T^*\psi)\rangle = \langle(-T\varphi, \varphi), (\psi, T^*\psi)\rangle = \langle -T\varphi, \psi\rangle + \langle \varphi, T^*\psi\rangle \ . \tag{3.70}$$

Since $\langle \varphi, T^*\psi\rangle = \langle T\varphi, \psi\rangle$, we get $\langle -T\varphi, \psi\rangle + \langle \varphi, T^*\psi\rangle = \langle -T\varphi, \psi\rangle + \langle T\varphi, \psi\rangle = 0$. This clearly forces $(\psi, T^*\psi) \in V(\Gamma(T))^\perp$. Conversely, suppose $(\psi, \eta) \in V(\Gamma(T))^\perp$. Then, we must have $0 = \langle V(\varphi, T\varphi), (\psi, \eta)\rangle = \langle -T\varphi, \psi\rangle + \langle \varphi, \eta\rangle$ for any $\varphi \in D(T)$. This implies

$$\langle \psi, T\varphi\rangle = \langle \eta, \varphi\rangle \ . \tag{3.71}$$

In other words, $\psi \in D(T^*)$ and $\eta = T^*\psi \in Ran(T^*)$. Then $(\psi, \eta) \in \Gamma(T^*)$. Hence $V(\Gamma(T))^\perp \subseteq \Gamma(T^*)$. This completes the proof of the first equality. Second equality immediately follows from the Proposition 3.50 (see for instance (Schmüdgen, 2012)). □

Now, we can give the proof of Theorem 3.49.

Proof of Theorem 3.49:

(i) We shall use the sequence definition of the closed operators given just after Definition 3.23. Let $\{\psi_m\}_{m=1}^\infty \in D(T^*)$ be a sequence converging to ψ in $\mathcal{H}$, and $\{T\psi_m\}_{m=1}^\infty$ converging to some vector χ in $\mathcal{H}$. Then, for any $\varphi \in D(T)$ dense in $\mathcal{H}$, we have $\langle \psi_m, T\varphi\rangle = \langle T^*\psi_m, \varphi\rangle \to \langle \psi, T\varphi\rangle = \langle \chi, \varphi\rangle$ as $m \to \infty$. This implies that $\psi \in D(T^*)$ and $T^*\psi = \chi$, so T^* is closed. □

Alternative proof of (i): It is just a simple corollary of the Proposition 3.51. Since $\Gamma(T)^\perp$ is closed thanks to the Lemma 3.4, and the range of unitary operators are closed, we get the desired result.

(ii) Since $\Gamma(T)$ is a linear subspace of $\mathcal{H} \times \mathcal{H}$, and using Corollary 3.7 we have $\overline{\Gamma(T)} = (\Gamma(T)^\perp)^\perp$. Using Proposition 3.51, we obtain

$$\overline{\Gamma(T)} = (\Gamma(T)^\perp)^\perp = (V^2\Gamma(T)^\perp)^\perp = (V(V\Gamma(T))^\perp)^\perp = (V\Gamma(T^*))^\perp \ .$$

Hence, if T^* is densely defined $T^{**} := (T^*)^*$ is well-defined and T is closable ($\Gamma(T) \subset \overline{\Gamma(T)} = (V\Gamma(T^*))^{\perp}$, which is always closed thanks to Lemma 3.4) and $\Gamma(\overline{T}) = \Gamma(T^{**})$.

Conversely, suppose that $D(T^*)$ is not dense so that there exists $0 \neq \psi \in D(T^*)^{\perp}$. Since $\langle(\psi, 0), (\varphi, T^*\varphi)\rangle = \langle\psi, \varphi\rangle + \langle 0, T^*\varphi\rangle = 0$, for all $\varphi \in D(T^*)$, $(\psi, 0) \in \Gamma(T^*)^{\perp}$. Then, $V(\Gamma(T^*)^{\perp})$ ($V(0, \psi) = (0, \psi)$) is not a graph of a linear operator due to Proposition 3.27. Since $\overline{\Gamma(T)} = (V\Gamma(T^*))^{\perp}$, T is not closable.

(iii) Using part (i), $T^* = \overline{T^*}$. Suppose now that T is closable. Using part (ii), we get

$$T^* = \overline{T^*} = (T^*)^{**} = T^{***} = (\overline{T})^* \ . \tag{3.72}$$

See for instance (Reed and Simon, 1972). □

Corollary 3.52 *If T is closable, then $T \subseteq T^{**}$.*

Corollary 3.53 *A symmetric operator is closable.*

Proof: For T is a symmetric operator, $T \subseteq T^*$ by Proposition 3.39 and T^* is densely defined from the proof given in (iii) in Proposition 3.39. Then, T is closable by Theorem 3.49 (ii). □

Corollary 3.54 *If T is symmetric, then $T \subseteq \overline{T} \subseteq T^*$.*

Proof: If T is symmetric, then it is closable from Corollary 3.53. Since the closure of T is the smallest closed extension of T, we get the desired inclusion result.

Proposition 3.55 *If T is symmetric, then $\overline{T}$ is symmetric.*

Proof: Suppose T is a symmetric operator, then Proposition 3.39 (iii) implies that $T^{**} \subseteq T^*$. From the definition of extension we have $T^{**}\varphi = T^*\varphi$ for all $\varphi \in D(T^{**})$. Then, since $\overline{T} = T^{**}$ for a densely defined T^* we obtain

$$\langle\psi, \overline{T}\varphi\rangle = \langle\psi, T^{**}\varphi\rangle \quad = \quad \langle\psi, T^*\varphi\rangle = \langle T^{**}\psi, \varphi\rangle = \langle\overline{T}\psi, \varphi\rangle \ .$$

for any $\varphi, \psi \in D(\overline{T})$. That is $\overline{T}$ is symmetric (see for instance (Schuller, 2016)). □

Remark 3.56 *Symmetry of T does not imply symmetry of T^*.*

Corollary 3.57 *If T^* is a densely defined linear operator on $\mathcal{H}$, and $z \in \mathbb{C}$, then*

$$\mathcal{H} = Ker(T^* - \bar{z}I) \oplus \overline{Ran(T - zI)} = Ker(\overline{T} - zI) \oplus \overline{Ran(T^* - \bar{z}I)} \ . \tag{3.73}$$

Proof: Since T^* is densely defined, one can replace T by T^* in Proposition 3.41 to get

$$Ker(\overline{T}) = Ran(T^*)^{\perp} \ , \tag{3.74}$$

which implies

$$\mathcal{H} = Ker(T^*) \oplus \overline{Ran(T)} = Ker(\overline{T}) \oplus \overline{Ran(T^*)} \ . \tag{3.75}$$

by the same argument used in the Corollary 3.42. Then, replacing T by $T - zI$, and using the facts $(T - zI)^* = T^* - \overline{z}I$, $\overline{(T - zI)} = (T - zI)^{**} = (T^* - \overline{z}I)^* = (\overline{T} - zI)$, the assertion follows. □

Corollary 3.58 *If T is self-adjoint, then T is closed.*

Proof: As a result of Theorem 3.49, $T = T^*$ is closed. □

Theorem 3.59 *(i) Suppose T has an inverse ($Ker(T) = \{0\}$) and $Ran(T)$ is dense in $\mathcal{H}$. Then T^* has an inverse and*

$$(T^*)^{-1} = (T^{-1})^* \ . \tag{3.76}$$

(ii) If T has an inverse, then T is closed if and only if T^{-1} is closed.

Proof: (i) Using the assumption that $Ran(T)$ is dense in $\mathcal{H}$ and by Proposition 3.41, we have $Ker(T^*) = Ran(T)^{\perp} = \{0\}$. Then $(T^*)^{-1}$ exists in its natural domain domain $Ran(T^*)$. Since $D(T^{-1}) = Ran(T) = \mathcal{H}$, $(T^{-1})^*$ is well-defined. Replacing T by T^{-1}

in Proposition 3.51, we get

$$\Gamma((T^{-1})^*) = V(\Gamma(T^{-1})^{\perp}) \ . \tag{3.77}$$

On the other hand, using the definition of V and V^{-1}, given in Equation (3.64), we obtain

$$-V^{-1}(\varphi, T\varphi) = -(T\varphi, -\varphi) = (-T\varphi, \varphi) = V(\varphi, T\varphi) \ . \tag{3.78}$$

Therefore

$$\Gamma((T^{-1})^*) = -V^{-1}(\Gamma(T^{-1})^{\perp}) \ . \tag{3.79}$$

Next, using Equation (3.67), Proposition 3.51 and Equation (3.66), we get

$$\begin{aligned}
\Gamma((T^*)^{-1}) &= U^{-1}(\Gamma(T^*)) = U^{-1}(V(\Gamma(T)^{\perp})) = U^{-1}V(\Gamma(T)^{\perp}) \\
&= V^{-1}U(\Gamma(T)^{\perp}) = V^{-1}(U(\Gamma(T))^{\perp}) = (-V^{-1})(\Gamma(T^{-1})^{\perp}) \ .
\end{aligned}$$

Hence, $\Gamma((T^*)^{-1}) = \Gamma((T^{-1})^*)$, or $(T^*)^{-1} = (T^{-1})^*$.

(ii) This is just a consequence of the Equation (3.67) since the range of unitary operators are closed (see for instance (Schmüdgen, 2012)). □

Remark 3.60 *As we have emphasized before that the necessary conditions for a linear operator T to be invertible are $Ker(T) = \{0\}$ and $Ran(T) = \mathcal{H}$. These conditions become sufficient conditions for particular classes of operators: 1) closed operators defined on entire $\mathcal{H}$ (Suppose T is closed on entire $\mathcal{H}$, $Ker(T) = \{0\}$, and $D(T^{-1}) = \mathcal{H}$. Then, T is invertible due to T^{-1} is also closed (thanks to 3.59) and the Closed Graph Theorem 3.25). 2) symmetric operators defined on entire $\mathcal{H}$ (Suppose $Ker(T) = \{0\}$ and T is symmetric, then T^{-1} is also symmetric, as shown previously. Thanks to the assumption $D(T^{-1}) = \mathcal{H}$, T is invertible due to Hellinger-Toeplitz Theorem 3.37).*

Corollary 3.61 *If T is a self-adjoint operator and its inverse exists, then T^{-1} is also a self-adjoint operator.*

Proof: Since $T = T^*$, and from the fact that T has an inverse, we have $Ran(T)^\perp = Ker(T^*) = Ker(T) = \{0\}$. This means that $Ran(T)$ is dense so that Theorem 3.59 (i) leads to the conclusion that $(T^*)^{-1} = T^{-1} = (T^{-1})^*$. $\square$

CHAPTER 4

RESOLVENT AND SPECTRUM OF AN OPERATOR

In order to describe our model introduced in the introduction, we need to use the so-called resolvent of operators. For this reason, we shall discuss this notion and its relation with the spectrum of operators.

4.1. Regularity Domains and Deficiency Index

Definition 4.1 *Let T be a linear operator. If there exists a number $c_z > 0$ such that*

$$||(T - zI)\varphi|| \geq c_z||\varphi|| \; , \tag{4.1}$$

for all $\varphi \in D(T)$, then we say that $z \in \mathbb{C}$ is a regular point for T. The set of all regular points of T is the regularity domain of T. The set of all regular points are denoted by $\pi(T)$.

Remark 4.2 *Unfortunately, the symbol for the regularity domain is not standard. Different books choose different notations. We shall stick to the notation used in (Schmüdgen, 2012).*

Lemma 4.3 *Let T be a symmetric operator on $\mathcal{H}$. Then, $\mathbb{C} \setminus \mathbb{R} \subseteq \pi(T)$.*

Proof: Let $z = \lambda + i\mu$, where $\lambda, \mu \in \mathbb{R}$. Using the property of symmetric operator given in Proposition 3.38 we have the following estimate $||(T - zI)\varphi|| \geq |\operatorname{Im} z|||\varphi||$ for all $\varphi \in D(T)$ and $z \in \mathbb{C}$. Hence, $z \in \pi(T)$ as long as $\operatorname{Im}(z) \neq 0$ (see for instance (Schmüdgen, 2012)). □

Definition 4.4 *We call the linear susbspace $Ran(T - zI)^{\perp}$ of $\mathcal{H}$ as the deficiency subspace of T where $z \in \pi(T)$, and its dimension (cardinality of an orthonormal basis of $\mathcal{H}$),*

$$d_z(T) := dim(Ran(T - zI)^{\perp}) \; , \tag{4.2}$$

is called the defect number of T at the point z.

Remark 4.5 *For a densely defined linear operator T, we have*

$$d_z(T) = dim(Ker(T^* - \overline{z}I)) \;, \tag{4.3}$$

thanks to the Proposition 3.41. In other words, the deficiency subspace $Ran(T - zI)^\perp$ for a densely defined linear operator T coincides with the eigenspace of its adjoint corresponding to the eigenvalue $\overline{z}$.

Proposition 4.6 *(Schmüdgen, 2012)*

Let T be a linear operator on $\mathcal{H}$, and $z \in \mathbb{C}$.

(i) *$z \in \pi(T)$ if and only if $T - zI$ has a bounded inverse $(T - zI)^{-1}$ on $Ran(T - zI)$. In this case*

$$||(T - zI)\varphi|| \geq c_z||\varphi|| \;, \tag{4.4}$$

where $c_z = ||(T - zI)^{-1}||^{-1}$.

(ii) *$\pi(T)$ is an open subset of $\mathbb{C}$. More precisely, if $z_0 \in \pi(T)$, $z \in \mathbb{C}$, and $|z - z_0| < c_{z_0}$, where c_{z_0} is the constant satisfying (4.1) for z_0, then $z \in \pi(T)$.*

(iii) *If T is closable, then $Ran(T - zI) = \overline{Ran(T - zI)}$ in $\mathcal{H}$, $\pi(\overline{T}) = \pi(T)$, and $d_z(\overline{T}) = d_{\overline{z}}(T)$ for $z \in \pi(T)$.*

(iv) *If T is closed and $z \in \pi(T)$ then $Ran(T - zI)$ is a closed linear subspace of $\mathcal{H}$.*

Proof: (i) ($\Rightarrow$) Suppose $z \in \pi(T)$ and $\varphi \in Ker(T - zI)$, then $(T - zI)\varphi = 0$. Since $z \in \pi(T)$, there exists $c_z > 0$ such that $0 = ||(T - zI)\varphi|| \geq c_z||\varphi||$, which implies that $\varphi = 0$. Therefore $Ker(T - zI) = \{0\}$. So $T - zI$ has an inverse. Then for any $\psi \in Ran(T - zI)$ there exists $\varphi \in D(T)$ such that $\varphi = (T - zI)^{-1}\psi$. Then, for $z \in \pi(T)$ we have $||(T - zI)^{-1}\psi|| \leq c_z^{-1}||\psi||$.

($\Leftarrow$) We assume $T - zI$ has a bounded inverse which is defined on $Ran(T - zI)$. Using the same definition of φ and ψ, we find

$$||\varphi|| \;\; = \;\; ||(T - zI)^{-1}\psi|| \leq ||(T - zI)^{-1}||||\psi||. \tag{4.5}$$

Hence we have

$$||(T - zI)\varphi|| \geq \underbrace{||(T - zI)^{-1}||^{-1}}_{=c_z} ||\varphi||. \tag{4.6}$$

(ii) Let us choose an arbitrary point $z_0 \in \pi(T)$, and $z \in \mathbb{C}$. Furthermore, assume $|z - z_0| < c_{z_0}$ where c_{z_0} is a constant such that the inequality (4.1) holds. Our aim is to find an another constant c_z satisfying (4.1). We begin with norm of $(T - zI)\varphi$, then adding and subtracting $z_0 I\varphi$ and using the reverse triangle-inequality, we get

$$\begin{aligned} ||(T - zI)\varphi|| &= ||(T - z_0 I)\varphi - (z_0 - z)\varphi|| \,, && (4.7) \\ &\geq \left| \underbrace{||(T - z_0 I)\varphi||}_{\geq c_{z_0}} - |z - z_0| ||\varphi|| \right| , && (4.8) \\ &\geq \underbrace{\left| \left| c_{z_0} ||\varphi|| - |z - z_0| ||\varphi|| \right| \right|}_{= \underbrace{\left(c_{z_0} - |z - z_0| \right)}_{:= c_z > 0} ||\varphi|| \,.} , && (4.9) \end{aligned}$$

(iii) First we show $\overline{Ran(T - zI)} \subseteq Ran(\overline{T} - zI)$.

Let $y \in \overline{Ran(T - zI)}$, then by the definition of closure there exists a sequence $\{\varphi_m\}_{m=1}^{\infty}$ in $D(T - zI) = D(T)$ such that $\psi_m := (T - zI)\varphi_m \to \psi$ as $m \to \infty$ in $\mathcal{H}$. Since z is a regular point there exists $c_z > 0$ such that

$$\begin{aligned} ||(T - zI)(\varphi_m - \varphi_l)|| &\geq c_z ||\varphi_m - \varphi_l|| && (4.10) \\ ||\psi_m - \psi_l|| &\geq c_z ||\varphi_m - \varphi_l|| \,. && (4.11) \end{aligned}$$

Then, the sequence $\{\varphi_m\}$ is Cauchy since $\{\psi_m\}$ is Cauchy. Let $\varphi := \lim_{m\to\infty} \varphi_m$, then $\lim_{m\to\infty} T\varphi_m = \lim_{m\to\infty} (\psi_m + z\varphi_m) = \psi + z\varphi$. Since T is closable, there exists a closed extension for T. We simply choose the smallest one, namely its closure $\overline{T}$ ($T\varphi_m = \overline{T}\varphi_m$ for all $\varphi_m \in D(T) \subseteq D(\overline{T})$). Then, $\varphi \in D(\overline{T})$ and $\overline{T}\varphi = \psi + z\varphi$. So $\psi = (\overline{T} - zI)\varphi$. That is $\psi \in Ran(\overline{T} - zI)$, which proves $\overline{Ran(T - zI)} \subseteq Ran(\overline{T} - zI)$.

Next, we will show $Ran(\overline{T} - zI) \subseteq \overline{Ran(T - zI)}$. let $\psi \in Ran(\overline{T} - zI)$, then there exists $\varphi \in D(\overline{T})$ such that $\psi = \overline{T}\varphi - z\varphi$. Since $\varphi \in D(\overline{T})$, there exists a sequence

$\{\varphi_m\}_{m=1}^{\infty} \in D(T)$ such that $\varphi_m \to \varphi$ and $T\varphi_m \to \psi + z\varphi$. Then

$$\psi = \lim_{m\to\infty} (T - zI)\varphi_m \;, \tag{4.12}$$

i.e., $\psi \in \overline{Ran(T - zI)}$. Hence $Ran(\overline{T} - zI) = \overline{Ran(T - zI)}$. They will have the same orthogonal complement, i.e., $Ran(\overline{T} - zI)^{\perp} = \overline{Ran(T - zI)}^{\perp}$. Using the above equality, we have

$$\begin{aligned} d_z(\overline{T}) &= dim\left[Ran(\overline{T} - zI)^{\perp}\right] = dim\left[\overline{Ran(T - zI)}^{\perp}\right] \\ &= dim\left[Ran(T - zI)^{\perp\perp\perp}\right] = dim\left[\overline{Ran(T - zI)^{\perp}}\right] \\ &= dim\left[Ran(T - zI)^{\perp}\right] = d_z(T) \;. \end{aligned}$$

It remains to show that $\pi(T) = \pi(\overline{T})$. Let $z \in \pi(T)$, then there exists $c_z > 0$ such that $||(T - zI)\varphi|| \geq c_z||\varphi||$ for all $\varphi \in D(T)$. Since $T \subseteq \overline{T}$, $T\varphi = \overline{T}\varphi$ for all $\varphi \in D(T)$. Our aim is to show $||(\overline{T} - zI)\phi|| \geq c_z||\phi||$ for all $\phi \in D(\overline{T})$. Let $\phi \in D(\overline{T})$, then there exists a sequence $\{\varphi_m\}_{m=1}^{\infty} \in D(T)$ such that $\varphi_m \to \phi$ and $T\varphi_m \to \psi + z\phi$. Since $z \in \pi(T)$ and $\varphi_m \in D(T)$, we have

$$||\underbrace{(T - zI)\varphi_m}_{=(\overline{T}-zI)\varphi_m}|| \geq c_z||\varphi_m|| \;. \tag{4.13}$$

Letting $m \to \infty$ and using the continuity of norm, we get $||(\overline{T} - zI)\phi|| \geq c_z||\phi||$ for all $\phi \in D(\overline{T})$, that is $z \in \pi(\overline{T})$.

Conversely, let $z \in \pi(\overline{T})$, then there exists $c_z > 0$ such that $||(\overline{T} - zI)\phi|| \geq c_z||\phi||$ for all $\phi \in D(\overline{T}) \supseteq D(T)$. Therefore the statement is true for all $\varphi \in D(T)$, and since $\overline{T}\varphi = T\varphi$ for all $\varphi \in D(T)$, we have $||(T - zI)\varphi|| = ||(\overline{T} - zI)\varphi|| \geq c_z||\varphi||$ for all $\varphi \in D(T)$. Therefore $z \in \pi(T)$. Hence $\pi(T) = \pi(\overline{T})$.

(iv) Suppose T is closed and $z \in \pi(T)$. Since T is closed, we have $T = \overline{T}$ by Proposition 3.30. Therefore Proposition 4.6 (iii) implies $\overline{Ran(T - zI)} = Ran(\overline{T} - zI) = Ran(T - zI)$, that is, $Ran(T - zI)$ is closed. □

Corollary 4.7 *If T is a closable densely defined linear operator, and $z \in \pi(T)$, then*

$$\mathcal{H} = Ker(T^* - \overline{z}I) \oplus Ran(\overline{T} - zI) \; . \tag{4.14}$$

Proof: Since $z \in \pi(T)$, Proposition 4.6(iii) implies that $Ran(\overline{T} - zI)$ is closure of $Ran(T - zI)$. Thus, combining this result with the Equation (3.73), we get the above result (see for instance (Schmüdgen, 2012)). □

Lemma 4.8 *If $\mathcal{F}$ and $\mathcal{G}$ are closed linear subspaces of a Hilbert space $\mathcal{H}$ such that $dim\,\mathcal{F} < dim\,\mathcal{G}$, then there exists a nonzero vector $y \in \mathcal{G} \cap \mathcal{F}^{\perp}$.*

Proof: First we suppose $dim\,\mathcal{F} = k$ and M is a closed linear subspace of $\mathcal{G}$ with $k+1$ dimension. Consider projection operators $P_M\psi := \sum\limits_{m=1}^{k+1} e_m\langle\psi, e_m\rangle$ and $P_{\mathcal{F}}\psi := \sum\limits_{m=1}^{k} e_m\langle\psi, e_m\rangle$ where $\{e_m\}_{m=1}^{k}$ and $\{e_m\}_{m=1}^{k+1}$ are orthonormal bases for $\mathcal{F}$ and M respectively. Then

$$P_M\psi = P_{\mathcal{F}}\psi + e_{k+1}\langle\psi, e_{k+1}\rangle \; . \tag{4.15}$$

Hence we choose $y = e_{k+1} \in M \subseteq \mathcal{G}$ and $\langle e_{k+1}, e_m\rangle = 0$ for any $m = 1, 2, \ldots, k$. That is $y = e_{k+1} \in \mathcal{G} \cap \mathcal{F}^{\perp}$.

Now we suppose $dim\mathcal{F}$ is infinite. Since $\mathcal{H}$ is separable, it has countable orthonormal basis and so does subspace of $\mathcal{H}$. Let $\{f_l : k \in L\}$ and $\{g_k : k \in K\}$ be orthonormal bases for $\mathcal{F}$ and $\mathcal{G}$, respectively. We define $L_k := \{g_l : \langle f_k, g_l\rangle\}$ where $k \in K$ and $L' = \bigcup\limits_{k\in K} L_k$. For any $k \in K$ the set L_k is again countable since L_k is a subset of a countable set $\{g_l : l \in L\}$ and having the same cardinality of natural numbers, i.e., $|L_k| = |\mathbb{N}|$. Also we have $dim\mathcal{F} = |K|$ is infinite. Therefore

$$\begin{aligned} |L'| &= |\bigcup_{k\in K} L_k| & (4.16)\\ &\leq |\mathbb{N}|\,|K| = |K| \; . & (4.17) \end{aligned}$$

The main assumption assumption $|K| = dim\,\mathcal{F} < dim\,\mathcal{G} = |L|$ and the above inequality lead us to $L' \leq L$. Then there exists an element $l \in L\backslash L'$ such that g_l belongs to basis of $\mathcal{G}$ which is orthogonal to f_k which belongs to basis of $\mathcal{F}$ for each $k \in K$. Hence $g_l \in \mathcal{G} \cap \mathcal{F}^{\perp}$ (see for instance (Schmüdgen, 2012)). □

A rather remarkable property of the defect numbers is that they are invariant under the changes of z:

Proposition 4.9 *Suppose that T is closable linear operator on $\mathcal{H}$. Then the defect number $d_z(T)$ is constant on each component of the open set $\pi(T)$.*

Proof: Since T is closable operator on $\mathcal{H}$, we have $d_z(T) = d_z(\overline{T})$, $\pi(T) = \pi(\overline{T})$ by Proposition 4.6 (iii). Then using Proposition 4.6 (iv), $Ran(T - \mu I)$ is closed for all $\mu \in \pi(T)$. Let us define $K_\mu := Ran(T - \mu I)^{\perp}$, then Corollary 3.7 gives $K_\mu^{\perp} = \overline{Ran(T - \mu I)} = Ran(T - \mu I)$, where $\mu \in \pi(T)$. Assume $z_0 \in \pi(T)$ and $z \in \mathbb{C}$ such that $|z - z_0| < c_{z_0}$. Thanks to Proposition 4.6 (iii), all complex numbers z with the above condition belongs to $\pi(T)$. Our aim is to show $d_z(T) = d_{z_0}(T)$. Suppose $d_z(T) < d_{z_0}(T)$. Then Lemma 4.8 implies that there exists a nonzero vector $\psi \in K_{z_0} \cap K_z^{\perp}$. In other words, $\psi \in Ran(T - z_0 I)^{\perp}$ such that $\psi \in \overline{Ran(T - zI)} = Ran(T - zI)$. This means that $\psi = (T - zI)\varphi$ for some nonzero $\varphi \in D(T)$. Since we must also have $\psi \in Ran(T - z_0 I)^{\perp}$. Therefore

$$\langle (T - zI)\varphi, (T - z_0 I)\varphi \rangle = 0\,. \tag{4.18}$$

Since the equation is symmetric in z and z_0, if we had assumed $d_{z_0}(T) < d_z(T)$ we would have got

$$\langle (T - z_0 I)\varphi, (T - zI)\varphi \rangle = 0\,. \tag{4.19}$$

In both cases, we have

$$\begin{aligned}
\langle (T - z_0 I)\varphi, (T - z_0 I)\varphi \rangle &= \langle (T - z_0 I + zI - zI)\varphi, (T - z_0 I)\varphi \rangle \\
&= \langle (T - zI)\varphi + (z - z_0)\varphi, (T - z_0 I)\varphi \rangle \\
&= \underbrace{\langle (T - zI)\varphi, (T - z_0 I)\varphi \rangle}_{=0} + \langle (z - z_0)x, (T - z_0 I)\varphi \rangle \\
&\leq |z - z_0|\, ||\varphi||\, ||(T - z_0 I)\varphi||\,,
\end{aligned}$$

where we have used Cauchy-Schwarz inequality (3.3). Hence we get

$$||(T - z_0 I)\varphi|| \leq |z - z_0| \; ||\varphi|| \; . \tag{4.20}$$

On the other hand, combining the above result with the fact that $z_0 \in \pi(T)$, that is, $c_{z_0}||\varphi|| \leq ||(T - z_0 I)\varphi||$, we must have

$$c_{z_0}||\varphi|| \leq ||(T - z_0 I)\varphi|| \leq |z - z_0| \; ||\varphi|| \tag{4.21}$$

which contradicts with the assumption $|z - z_0| < c_{z_0}$. Hence $d_{z_0}(T) = d_z(T)$ in the disc $|z - z_0| < c_{z_0}$. In other words, $d_z(T)$ is locally constant.

It remains to show that this constant is the same constant all over the connected (the space X is said to be connected if there does not exist a pair of disjoint nonempty open subsets of X such that their union is X) component of the open set $\pi(T)$ in the complex plane. This can be proved by using the well-known argument in topology. Let U be a connected component of open set $\pi(T)$ and α and β be any two points in the same connected component U. Then there exists a polygonal path P in U from α to β (existence of such a polygonal is guaranteed by a theorem and it is a very useful characterization of connected sets on a complex plane. Here we have skipped to prove it, see (Ahlfors, 1979) for the details). The polygonal path can be defined on a compact interval $[0, 1]$ so that its image is compact since the continuous map of a compact set is again compact (Ahlfors, 1979).

Then, we define for each point z in the polygonal path P

$$U_z = \{z' \in \mathbb{C} : |z' - z| < c_z\} \; . \tag{4.22}$$

Then $\{U_z : z \in P\}$ is an open cover of the compact set P, so there exists a finite subcover $\{U_{z_m}\}_{m=1}^{N}$ of P so that $\cup_{m=1}^{N} U_{z_m} = P$. Since $d_z(T)$ is constant for each disc, we find $d_\alpha(T) = d_\beta(T)$ for any $\alpha, \beta \in U$. See for instance (Schmüdgen, 2012). □

Remark 4.10 *The above theorem holds for nonclosable operators as well but the proof* *is much harder (see (Berezansky et al., 1996) for the details).*

As we all know from linear algebra that one of most important characteristics of linear operators, or matrices, is their eigenvalues. A nonzero vector φ in a finite dimensional vector space V is an *eigenvector* of the linear operator A (its matrix elements are $(a_{ij})_{i,j=1}^{N}$) which corresponds to an *eigenvalue* $\lambda \in \mathbb{C}$ if $A\varphi = \lambda\varphi$. The collection of all eigenvalues of the operator A is called its *spectrum*, denoted by $\sigma(A)$. Rewriting $A\varphi = \lambda\varphi$ as $(A - \lambda I)\varphi = 0$, we have

$$\lambda \in \sigma(A) \Leftrightarrow A - \lambda I \text{ is singular} \Leftrightarrow \det(A - \lambda I) = 0 \ , \tag{4.23}$$

and $\{\varphi \neq 0 : \varphi \in Ker(A - \lambda I)\}$ is the set of all eigenvectors associated with λ. $Ker(A - \lambda I)$ is called the eigenspace for A. To put it an another way, if $\lambda \notin \sigma(A)$, then $(A - \lambda I)$ is invertible or $Ker(A - \lambda I) = \{0\}$.

One can also generalize the above notion of the spectrum of a linear operator to infinite dimensional vector spaces, in particular to Hilbert spaces. We can still talk about the eigenvalues of an operator similarly but one must be very careful. The direct generalization of the above notion of the spectrum is not so trivial as the following example shows. Consider once again the position operator X defined on its natural domain given in Example 3.19. The eigenvalue of this operator must satisfy

$$(X\psi)(x) = x\psi(x) = \lambda\psi(x) \ , \tag{4.24}$$

which implies that $\psi(x)$ would be equal to zero almost everywhere, so it is the zero function in $L^2(\mathbb{R})$. Therefore, the position operator X defined on $L^2(\mathbb{R})$ has no eigenvalues so its spectrum is empty set if we would like to stick the finite dimensional definition of the spectrum (position operator indeed admits so called generalized eigenvectors, which are generalized functions, namely $\delta(x - \lambda)$ (Appel, 2007)). This part of the spectrum can also be considered as the approximate in the sense that there exists a sequence $\psi_m \in D(X) \neq 0$ such that $\lim_{m\to\infty} \frac{||(X-\lambda I)\psi_m||}{||\psi_m||} = 0$. We refer the reader to (Hall, 2013).

We shall give a natural definition of the spectrum of an operator in infinite dimensional vector spaces, and unfortunately it will be defined indirectly, so we first define those points of complex plane which are not in the spectrum by drawing an analogy with the finite dimensional vector spaces described above. For this purpose, we shall define the inverse operator $(T - zI)^{-1}$ for a particular class of operators.

4.2. Resolvent

Definition 4.11 *The resolvent set $\rho(T)$ of a closed operator T is a set of points $z \in \mathbb{C}$ for which $T - zI$ has a bounded inverse defined everywhere on $\mathcal{H}$ and the inverse $(T - zI)^{-1}$ is called resolvent of T at z, from $\mathcal{H}$ onto $D(T)$, and denoted by $R_z(T)$, i.e.,*

$$R_z(T) := (T - zI)^{-1} . \tag{4.25}$$

The set $\sigma(T) = \mathbb{C} \setminus \rho(T)$ is called the spectrum of the linear operator T.

Remark 4.12 *Resolvent is also defined as $R_z(T) := (zI - T)^{-1}$ in the literature. Moreover, if $T - zI$ is a bijection of $D(T)$ onto $\mathcal{H}$. It is immediate to see that $T - zI$ is bijective if and only if the inverse $(T - zI)^{-1}$ exists and defined on the whole $\mathcal{H}$. The only task we must show is that $(T - zI)^{-1}$ is bounded if $(T - zI)$ is bijective. Since we assume that T is closed, so is $T - zI$. Hence, $(T - zI)^{-1}$ is closed by Theorem 3.59. In other words, $(T - zI)^{-1}$ is a closed linear operator on the entire $\mathcal{H}$, so that it must be bounded by closed graph theorem (Theorem 3.25).*

Remark 4.13 *Actually, one can also define the spectrum of not necessarily closed operators. Suppose $z \in \rho(T)$, then $(T - zI)^{-1}$ is bounded everywhere (by definition). Since bounded operators are closed, $(T - zI)^{-1}$ is closed and its inverse $T - zI$ or T must also be closed by Theorem 3.59. What this means that we get a contradiction if T is not closed so $\rho(T) = \varnothing$ and $\sigma(T) = \mathbb{C}$. For this reason, we only consider the spectrum of closed operators.*

Proposition 4.14 *Let T be a closed operators on $\mathcal{H}$. Then, we have*

(i) $\rho(T) = \{z \in \pi(T) \ : d_z(T) = 0\}$.

(ii) $\rho(T)$ *is an open subset, and* $\sigma(T)$ *is a closed subset of* $\mathbb{C}$.

Proof: (i) Suppose $z \in \pi(T)$ such that $d_z(T) = 0$. Since $z \in \pi(T)$,

$$(T - zI)^{-1} : Ran(T - zI) \to D(T) \text{ is bounded} \tag{4.26}$$

thanks to Proposition 4.6. Since T is closed, then $Ran(T - zI)$ is a closed linear subspace of $\mathcal{H}$ by Proposition 4.6 (iv). Then

$$\mathcal{H} = Ran(T - zI) \oplus Ran(T - zI)^{\perp} . \tag{4.27}$$

On the other hand, since $0 = d_z(T) = dim\left(Ran(T - zI)^{\perp}\right)$, then $Ran(T - zI) = \mathcal{H}$. Therefore $(T - zI)^{-1}$is bounded on $\mathcal{H}$, i.e., $z \in \rho(T)$.

Conversely, let $z \in \rho(T)$, then $(T - zI)^{-1}$ is bounded on $\mathcal{H}$. That is

$$D\left((T - zI)^{-1}\right) = Ran(T - zI) = \mathcal{H} .$$

Therefore we get $Ran(T - zI)^{\perp} = \{0\}$ by Equation (4.27). That is $d_z(T) = 0$. To show $z \in \pi(T)$ we use invertiblity of $T - zI$. Since $T - zI$ is invertible, there exists $c > 0$ such that

$$||(T - zI)^{-1}\psi|| \leq c||\psi|| , \tag{4.28}$$

for any $\psi \in \mathcal{H} = Ran(T - zI)$. Therefore there exists $\varphi \in D(T)$ such that $\psi = (T - zI)\varphi$, then

$$\begin{aligned} ||(T - zI)^{-1}(T - zI)\varphi|| &\leq c||(T - zI)\varphi|| && (4.29)\\ ||\varphi|| &\leq c||(T - zI)\varphi|| , && (4.30) \end{aligned}$$

which implies $z \in \pi(T)$. Hence we proved (i).

(ii) Since $\pi(T)$ is open by Proposition 4.6 and $d_z(T)$ is locally constant on $\pi(T)$ by Proposition 4.9, previous result (i) also says that $\rho(T)$ is open. Therefore $\sigma(T) = \mathbb{C} \setminus \rho(T)$ is closed (see for instance (Schmüdgen, 2012)). □

We have two very useful identities about the resolvents of closed operators. One of them implies that $R_z(T)$ and $R_{z_0}(T)$ commutes for all $z_0, z \in \rho(T)$.

Proposition 4.15 (Resolvent identities) *Let T and S be two closed operator on $\mathcal{H}$ such that $D(S) \subseteq D(T)$ then we have*

(i) (First Resolvent identity-Hilbert identity)

$$R_z(T) - R_{z_0}(T) = (z - z_0)R_z(T)R_{z_0}(T) \ , \tag{4.31}$$

for $z, z_0 \in \rho(T)$.

(ii) (Second Resolvent identity)

$$R_z(T) - R_z(S) = R_z(T)(S - T)R_z(S) \ , \tag{4.32}$$

for $z \in \rho(T) \cap \rho(S)$.

Proof: We will first prove (ii): Suppose $z \in \rho(T) \cap \rho(S)$. For all $\psi \in \mathcal{H}$, we get

$$\begin{aligned} R_z(T)(S-T)R_z(S)\psi &= R_z(T)(S - zI + zI - T)R_z(S)\psi \\ &= R_z(T)((S - zI) - (T - zI))R_z(S)\psi \\ &= R_z(T)\left(\psi - (T - zI)R_z(S)\psi\right) \\ &= R_z(T)\psi - R_z(S)\psi \ . \end{aligned}$$

This proves Equation (4.32), which relates the resolvent of two different operators at the same point.

(i) We set

$$S := T + (z - z_0)I \ , \tag{4.33}$$

then

$$S - zI = T - z_0 I \ . \tag{4.34}$$

This implies that

$$R_z(S) = R_{z_0}(T) \ . \tag{4.35}$$

Therefore by the second part of the proposition and using the Equation (4.33) and (4.35), we get

$$\begin{aligned} R_z(T) - R_z(S) &= R_z(T)(T + (z - z_0)I - T)R_z(S) \\ R_z(T) - R_{z_0}(T) &= R_z(T)(z - z_0)R_{z_0}(T) \\ R_z(T) - R_{z_0}(T) &= (z - z_0)R_z(T)R_{z_0}(T) \ . \end{aligned}$$

This simply gives a relation between the resolvent of one operator at two different points. See for instance (Schmüdgen, 2012). □

There are some implications of these identities. First, the resolvent can be viewed as a function from set of complex numbers on its resolvent set to the bounded operators $\mathcal{L}(\mathcal{H})$. Furthermore, we have

Theorem 4.16 *The operator-valued function $R_z(T)$ has a derivative at every $z \in \rho(T)$, that is, the limit in the norm of $\mathcal{L}(\mathcal{H})$*

$$\lim_{h \to 0} \frac{1}{h} \left(R_{z+h}(T) - R_z(T) \right) := R'_z(T) \ , \tag{4.36}$$

exists for every $z \in \rho(T)$.

Proof: The proof is rather straightforward by writing the expression inside the bracket as $R_{z+h}(T)R_z(T)$ using the first resolvent identity (4.31). Then, this converges to $R_z^2(T)$ with respect to norm in $\mathcal{L}(\mathcal{H})$. □

In analogy with the complex analysis, we shall say that the operator-valued function resolvent $R_z(T)$ for a closed operators are analytic on their resolvent set $\rho(T)$. One can show that operator-valued function is analytic on some region if and only if the function constructed from the bounded linear functional l, by $F_{\varphi,l}(z) := l(F(z)\varphi)$ is analytic on the same region in the complex plane and $\varphi \in \mathcal{H}$, and $l \in \mathcal{H}'$ (dual space of $\mathcal{H}$) (Reed and Simon, 1972; Berezansky et al., 1996).

Furthermore, we have the following power series expansion of the resolvent:

Proposition 4.17 *Suppose that $z_0 \in \rho(T)$, $z \in \mathbb{C}$ and $|z - z_0| < ||R_{z_0}(T)||^{-1}$. Then we have $z \in \rho(T)$ and*

$$R_z(T) = \sum_{n=0}^{\infty} (z - z_0)^n R_{z_0}^{n+1}(T) \ , \tag{4.37}$$

where the series converges in the operator norm. In particular,

$$\lim_{z \to z_0} ||R_z(T) - R_{z_0}(T)|| = 0 \ \textit{for } z_0 \in \rho(T). \tag{4.38}$$

Proof: Since $z_0 \in \rho(T) \subseteq \pi(T)$, then Proposition 4.6 (i) implies that

$$||(T - z_0 I)\varphi|| \geq || \underbrace{(T - z_0 I)^{-1}}_{R_{z_0}(T)} ||^{-1} ||\varphi|| \ . \tag{4.39}$$

Thank to the assumption $|z - z_0| < ||R_{z_0}||^{-1}$, we have $d_z(T) = d_{z_0}(T) = 0$ and $z \in \rho(T) \subseteq \pi(T)$ by Proposition 4.9 and Proposition 4.14 (i). On the other hand, the assumption $|z - z_0| < ||R_{z_0}(T)||^{-1}$ also implies $||(z - z_0)R_{z_0}(T)|| < 1$. Then the operator $I - (z - z_0)R_{z_0}(T)$ has a bounded inverse which is defined on whole $\mathcal{H}$ by Proposition 3.47 as follows:

$$(I - (z - z_0)R_{z_0(T)})^{-1} = \sum_{m=0}^{\infty} (z - z_0)^m R_{z_0}^m(T) \ . \tag{4.40}$$

Using the first resolvent identity (Equation 4.31), we notice that

$$\begin{aligned} R_z(T)\,(I - (z - z_0)R_{z_0}(T)) &= R_z - (z - z_0)R_z(T)R_{z_0}(T) \ , \\ &= R_z(T) - (R_z(T) - R_{z_0}(T) \ , \\ &= R_{z_0}(T) \ . \end{aligned}$$

Therefore we get

$$R_z(T) = R_{z_0}(T)\left(I - (z - z_0)R_{z_0}(T)\right)^{-1} \ . \tag{4.41}$$

We multiply Equation (4.40) by $R_{z_0}(T)$ from the left and plugging into the Equation (4.41), we get

$$R_z(T) = \sum_{m=0}^{\infty}(z - z_0)^m R_{z_0}^{m+1}(T) \ . \tag{4.42}$$

This completes the proof of the Equation (4.37). Equation (4.38) is just the continuity of operator-valued analytic function $R_z(T)$ at $z = z_0$, which is just another consequence of the first resolvent identity. See for instance (Schmüdgen, 2012). □

A natural question may arise whether the resolvent set is empty or non empty for a given linear operator on $\mathcal{H}$. A partial answer is given by the following theorem:

Theorem 4.18 *Let T be a bounded linear operator on $\mathcal{H}$. Then $\sigma(T)$ is not empty.*

Proof: Suppose $\sigma(T) = \varnothing$. Then $\rho(T) = \mathbb{C}$ and the resolvent is an operator-valued entire function due to the Theorem 4.16. From the Proposition 4.17 $R_z(T)$ is also continuous in $\mathbb{C}$. Since norm is a continuous map, $||R_z(T)||$ is continuous in $\mathbb{C}$. It follows from Weierstrass extreme value theorem (Rudin, 1976) in analysis (continuous functions on compact space are bounded) that $||R_z(T)||$ is a bounded function on the disk $\overline{B(2||T||;0)}$. For those points $z \in \mathbb{C} \setminus \overline{B(2||T||;0)}$, we have $||R_z(T)|| = |z|^{-1}||\left(I - \frac{T}{z}\right)^{-1}|| \leq (2||T||^{-1})\left(1 - \frac{||T||}{z}\right)^{-1} < 2/|z|$, where we have used the fact that absolute convergence implies convergence in Banach space $\mathcal{L}(\mathcal{H})$. These show that $\sup_{z\in\mathbb{C}}||R_z(T)|| = c_1 < \infty$. Moreover, $||R_z(T)|| \to 0$ as $|z| \to \infty$. We consider now the numerical function with complex variable $f_{\varphi,l}(z) := l(R_z(T)\varphi)$. By definition, $f_{\varphi,l}(z)$ is an entire function since $R_z(T)$ is analytic operator-valued function. Since l is a bounded linear functional, we have $|f_{\varphi,l}(z)| \leq ||l||||R_z(T)\varphi|| \leq c||l||||\varphi||$. This implies that the function $f_{\varphi,l}$ is bounded on the entire complex plane. From the beautiful result in complex analysis, Liouville theorem (Ahlfors, 1979) states that every bounded entire function must be constant, i.e., $f_{\varphi,l}(z) = c_2$ for all $z \in \mathbb{C}$. From the decaying result of $||R_z(T)||$ given above, we should have $f_{\varphi,l}(z) = 0$ for all z. This forces us to conclude $l(R_z(T)\varphi) = 0$ so $R_z(T)\varphi = (T - zI)^{-1}\varphi = 0$ for all $\varphi \in \mathcal{H}$. However, this is a contradiction because $(T - zI)R_z(T) = I$ (see (Hislop and Sigal, 2012)). □

There are some important subsets of the spectrum. Recall that the resolvent set was defined as the set of points in a complex plane such that

(1) $(T - zI)^{-1}$ exists and

(2) $(T - zI)^{-1}$ is bounded on the whole Hilbert space $\mathcal{H}$.

It follows from the above conditions that they can be stated as

(1) $Ker(T - zI) = \{0\}$ and

(2) $(T - zI)^{-1}$ is bounded and $Ran(T - zI) = \mathcal{H}$.

As we have seen in the above eigenvalue problem (4.24) for the position operator example, its spectrum was an empty set. This forces us to weaken the definition of the spectrum for the operators defined on infinite dimensional spaces. The first subset of the spectrum is the case where the condition (1) does not hold:

Definition 4.19 *Let T be a closed linear operator then the set*

$$\sigma_p(T) = \{z \in \mathbb{C} : Ker(T - zI) \neq \{0\}\} \ , \tag{4.43}$$

is called the point spectrum of T. The elements of σ_p are eigenvalues of T, the dimension of $Ker(T - zI)$ is the multiplicity and the nonzero vectors $\psi \in Ker(T - zI)$ is called eigenvectors of T. Clearly these elements are poles of the operator-valued function, resolvent $(T - zI)^{-1}$.

We can remove the second condition in two forms while keeping the first condition (injectivity), in other words, we may release the surjectivity: one is weaker than the other one. We may have:

(i) The inverse $(T - zI)^{-1}$ exists but $(T - zI)^{-1}$ is not bounded on the entire $\mathcal{H}$. In this case, $Ran(T - zI)$ is not dense in $\mathcal{H}$. The set of all complex numbers $z \in \mathbb{C}$ for which $(T - zI)$ has a bounded inverse which is not defined not on the full $\mathcal{H}$ is called the *residual spectrum* of T, denoted by $\sigma_r(T)$.

(ii) The inverse $(T - zI)^{-1}$ exists but $(T - zI)^{-1}$ is not bounded on a densely defined subspace of $\mathcal{H}$. In this case, $\overline{Ran(T - zI)} = \mathcal{H} \neq Ran(T - zI)$, i.e., $Ran(T - zI)$ is not closed subspace of $\mathcal{H}$. The set of all complex numbers $z \in \mathbb{C}$ for which $(T - zI)^{-1}$ exists but not bounded on a densely defined subspace of $\mathcal{H}$ is called the *continuous spectrum* of T, denoted by $\sigma_c(T)$.

These subsets of the spectrum are in general not disjoint. Such a distinction between different subsets of the spectrum is also convenient from the physical point of view. They represent a different physical situation of the problem, such as, bound state and scattering states of a quantum mechanical system.

4.3. Basic Criteria for Self-Adjoint Operators and Their Spectrum

Since the dynamics in quantum mechanics must be generated by the self-adjoint operator H, namely the Hamiltonian, we must be sure that the formal Hamiltonian

$$H = T + V \tag{4.44}$$

is self-adjoint for a given system. However, it is rather difficult to check whether a given Hamiltonian is self-adjoint or not due to the technical domain issues. Nevertheless, we have one important simple criteria for self-adjointness:

Theorem 4.20 (The Basic Criteria For Self-Adjointness) *Let T be a symmetric operator on a Hilbert space. Then, the followings are equivalent:*

(i) *T is self adjoint.*

(ii) *T is closed and $Ker(T^* \pm iI) = \{0\}$.*

(iii) *$Ran(T \pm iI) = \mathcal{H}$.*

Proof: $(i) \implies (ii)$:

Suppose T is self-adjoint. T is closed from Corollary 3.58. Let $\psi \in D(T) = D(T^*)$ and suppose $T^*\psi = T\psi = \pm i\psi$. This gives

$$\pm i\langle\psi, \psi\rangle = \langle\psi, \pm i\psi\rangle = \langle\psi, T\psi\rangle = \langle T^*\psi, \psi\rangle = \langle\pm i\psi, \psi\rangle = \mp i\langle\psi, \psi\rangle \ , \tag{4.45}$$

which leads to $\psi = 0$, i.e., $Ker(T^* \pm iI) = \{0\}$.

$(ii) \implies (iii)$: Suppose that (ii) holds. Since $T^*\psi = \pm i\psi$ has no nontrivial solutions, Proposition 3.41 implies that $Ker((T \pm iI)^*) = Ker(T^* \mp iI) = Ran(T \pm iI)^\perp = \{0\}$, that is, $Ran(T \pm iI)$ is dense in $\mathcal{H}$.

It remains to show that $Ran(T \pm iI)$ is closed. Since T is assumed to be symmetric, Equation (3.42) implies $||(T \pm iI)\varphi||^2 = ||T\varphi||^2 + ||\varphi||^2 \geq ||\varphi||^2$ or $\pm i \in \pi(T)$. Hence, since T is closed by assumption $Ran(T \pm iI)$ is closed thanks to Proposition 4.6.

$(iii) \implies (i)$: Suppose $Ran(T - iI) = \mathcal{H}$ and let $\psi \in D(T^*)$, and $(T^* - iI)\psi = \eta$ where $\eta \in \mathcal{H}$. Since $T - iI$ is onto, there exists $\varphi \in D(T - iI) = D(T)$ such that $(T - iI)\varphi = \eta = (T^* - iI)\psi$. On the other hand, since T is symmetric operator, Proposition 3.39 implies

$$(T - iI)\varphi = (T^* - iI)\varphi \ , \tag{4.46}$$

for any $\varphi \in D(T) \subseteq D(T^*)$. Therefore we have

$$(T^* - iI)(\psi - \varphi) = 0 \ , \tag{4.47}$$

where $\psi - \varphi \in D(T^*)$. Using Proposition 3.41, we have $Ker(T^* - iI) = Ran(T + iI)^\perp = \{0\}$ (since $Ran(T + iI) = \mathcal{H}$). Therefore $\psi = \varphi \in D(T)$, that is $T^* \subseteq T$. Hence $T = T^*$. See for instance (Reed and Simon, 1975). $\square$

Remark 4.21 *The above criteria can also be stated for one point on the upper half plane and another one on the lower half plane thanks to the theorem, which we are going to state below. The reason why the above version is given lies in the fact that it is sufficient to pick the points as* $\pm i$.

Theorem 4.22 *Let* T *be a symmetric operator and* $Ran(T - zI) = \mathcal{H}$ *for some* z *with* $\mathrm{Im}(z) > 0$, *then it is true for every* z *with* $\mathrm{Im}(z) > 0$. *The same holds for* $\mathrm{Im}(z) < 0$. *Moreover, if* T *is a self-adjoint then* $T - zI$ *is invertible for every* z *with* $\mathrm{Im}(z) \neq 0$ *and satisfies*

$$||(T - zI)^{-1}|| \leq \frac{1}{|\mathrm{Im}(z)|} \ . \tag{4.48}$$

Proof: Suppose $Ran(T - zI) = \mathcal{H}$ and let us choose an arbitrary point in the complex plane with a positive imaginary part, i.e., $z = \lambda + i\mu$ where $\lambda \in \mathbb{R}$ and $\mu > 0$. Since T is symmetric operator, we are allowed to use Equation (3.42). Then we have $||(T -$

$zI)\varphi|| \geq |\mu|||\varphi||$ for any $\varphi \in D(T)$, which means $z \in \pi(T)$, then Proposition 4.6 (i) implies that $(T - zI)^{-1}$ exists and bounded on $Ran(T - zI)$. If we assume further that $Ran(T - zI) = \mathcal{H}$, $(T - zI)^{-1}$ is defined and bounded on the entire Hilbert space $\mathcal{H}$, so for any $\psi \in \mathcal{H}$, we have $\varphi = (T - zI)^{-1}\psi$, where $\varphi \in D(T)$. Then plugging φ in the above inequality we obtain

$$||(T - zI)^{-1}\psi|| \leq \frac{1}{|\mu|}||\psi|| , \tag{4.49}$$

for all $\psi \in \mathcal{H}$ and given particular point z. Our aim is now to show $(T - z'I)$ is also invertible as long as $\mathrm{Im}(z') > 0$. Using $T - z'I = (T - zI) + (z - z')I$ and the Theorem 3.48, $T - z'I$ is invertible for those z' such that $|z - z'| \, ||(T - zI)^{-1}|| < 1$.

This bound is guaranteed if we impose $|z - z'| < |\mu|$. This means, if we choose z' within this open disk, the operators $(T - z'I)$ will be invertible. So its range will be full $\mathcal{H}$. We begin with z then we choose z' such that $|z - z'| \leq |\mu|$ then our new z becomes z' with imaginary part μ', then we choose another z'' such that $|z' - z''| \leq |\mu'|$. We continue with this fashion throughout the whole complex upper half plane and extend the invertiblity to the for all z in the upper half plane, that is, $T - zI$ is invertible for all z with $\mathrm{Im}(z) > 0$, so that $Ran(T - z'I) = \mathcal{H}$ (similarly we can extend invertiblity to the lower half plane by starting on an arbitrary point in the lower half plane).

For the second part of the theorem, suppose T is self-adjoint, then we get $Ran(T \pm iI) = \mathcal{H}$ by Theorem 4.20. Hence by the first part of the theorem we have $T - zI$ is invertible and its inverse satisfies (4.48) for all z with $\mathrm{Im}(z) \neq 0$. See for instance (Gustafson and Sigal, 2011). □

Theorem 4.23 *The spectrum of a self-adjoint operator is a subset of real line.*

Proof: Let z be a complex number with $\mathrm{Im}(z) \neq 0$ and T be a self-adjoint operator. Our aim is to show $z \in \rho(T)$. Since T is self-adjoint, it is symmetric.

Then, Equation (3.42) implies $|\mathrm{Im}(z)|||\varphi|| \leq ||(T - zI)\varphi||$ for any $\varphi \in D(T)$, that is $z \in \pi(T)$. Therefore Proposition 4.6 (i) implies $T - zI$ has a bounded inverse on $Ran(T - zI)$. Thanks to Theorem 4.22 and Theorem 4.20, $Ran(T - zI) = \mathcal{H}$. Hence $(T - zI)$ is invertible (see (Dimock, 2011)). □

Lemma 4.24 *Let T be a self-adjoint operator on $\mathcal{H}$. Then, $\sigma_r(T) = \varnothing$.*

Proof: Let $z \in \sigma(T)$ such that $Ker(T - zI) = \{0\}$ (inverse $(T - zI)^{-1}$ exists). Then, it follows from Proposition 3.41 and Lemma 4.23 that $Ran(T - zI)^{\perp} = Ker(T^{*} - zI) = Ker(T - zI) = \{0\}$, which implies that $Ran(T - zI)$ is dense in $\mathcal{H}$, so that $z \notin \sigma_r(T)$ (see for instance (Schmüdgen, 2012)). □

For the unbounded operators, it is difficult to define the convergence since the norm of the unbounded operators is infinite. One idea is to define the convergence in terms of the bounded "functions" of these unbounded operators, which become useful later on (see (Reed and Simon, 1975)).

Definition 4.25 *Let $\{T_m\}_{m=1}^{\infty}$ be sequence of self-adjoint operators on $\mathcal{H}$ and T be a self-adjoint operator. Then, T_m is said to converge to T in the norm resolvent sense if $\lim\limits_{m\to\infty} ||R_z(T_m) - R_z(T)|| = 0$ for all z with $\operatorname{Im}(z) \neq 0$. T_m is said to converge to T in the strong resolvent sense if $\lim\limits_{m\to\infty} ||(R_z(T_m) - R_z(T))\varphi|| = 0$ for all $\varphi \in \mathcal{H}$ and z with $\operatorname{Im}(z) \neq 0$.*

CHAPTER 5

VON NEUMANN'S THEORY OF SELF-ADJOINT EXTENTIONS AND DIRAC DELTA POTENTIAL

In quantum mechanics, the heuristic arguments usually determine the Hamiltonian of the system, which can be easily chosen to be symmetric. However, the Hamiltonian operator must be self-adjoint as well, symmetry condition is not sufficient. The reason for imposing such a strong condition lies in the fact that we have the unitary time evolution of the system. Stone's theorem (Reed and Simon, 1975) guarantees that there is a one-to-one correspondence between self-adjoint operators and strongly continuous one-parameter groups of unitary operators $U = \exp(itH)$. Therefore, the determining of the self-adjoint extension of a given symmetric operator can not just be considered as just a mathematical technical detail.

There are various methods to define the point interaction in Quantum Mechanics. One way to do this is based on the idea of self-adjoint extensions of symmetric operators. In this chapter, we shall briefly discuss this method and give some examples.

5.1. The Cayley Transform of a Symmetric Operator

Let $C = \{z \in \mathbb{C} : |z| = 1\}$ be unit circle on the complex plane $\mathbb{C}$. Recall from complex analysis that Möbius transformation $w(t) = \frac{t-\lambda}{t-\overline{\lambda}}$ maps the real axis onto $C\backslash\{1\}$ and the upper half-plane onto the set inside of C, and it maps lower half-plane onto the set outside of C (Brown et al., 2009).

To see this, suppose $t = t_1 \in \mathbb{R}$. Then,

$$|w(t_1)|^2 = \frac{(t_1 - \lambda)(t_1 - \overline{\lambda})}{(t_1 - \overline{\lambda})(t_1 - \lambda)} = 1 \ . \tag{5.1}$$

This means that $w(t)$ sends t_1 to a point which belongs to the unit circle. But notice that $w(t_1) \neq 1$ in general since $\lambda \neq \overline{\lambda}$. Therefore we have shown that the transformation

$w(t)$ maps the straight line $\mathbb{R}$ to the unit circle C. Moreover, for any complex number

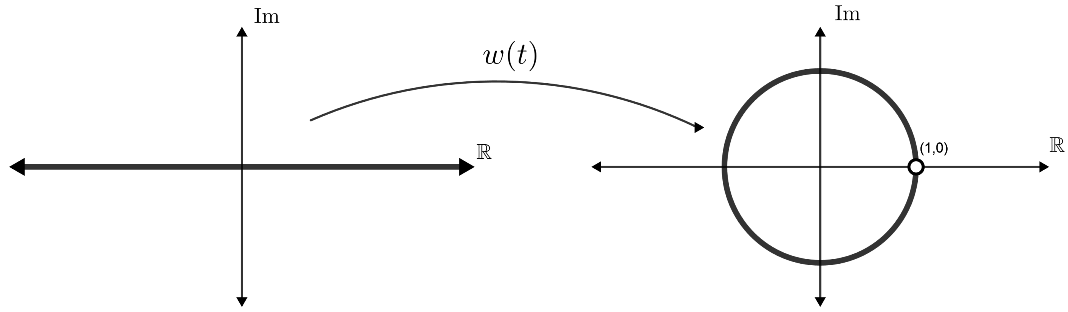

Figure 5.1. $w(t)$ sends the real axis to unit circle

$t = t_1 + it_2$ in upper half-plane, we have the following bound

$$|w(t)|^2 = \left|\frac{t_1 + it_2 - (\lambda_1 + i\lambda_2)}{t_1 + it_2 - (\lambda_1 - \lambda_2)}\right|^2 \tag{5.2}$$

$$= \left|\frac{(t_1 - \lambda_1) + i(t_2 - \lambda_2)}{(t_1 - \lambda_1) + i(t_2 + \lambda_2)}\right|^2 \tag{5.3}$$

$$= \frac{(t_1 - \lambda_1)^2 + (t_2 - \lambda_2)^2}{(t_1 - \lambda_1)^2 + (t_2 + \lambda_2)^2} < 1 \ , \tag{5.4}$$

if $t_2 > 0$. This means that $|w(t)| \leq 1$ represents a disk of radius 1. Hence we have shown that the transformation $w(t)$ maps the upper half-plane to the unit disk. If $t_2 < 0$, then $|w(t)| > 1$. This means that $w(t)$ maps maps the lower half-plane to the outside of the disk. The Cayley Transform is an operator analog of this transformation. It maps symmetric operators onto isometric operators V for which $Ran(I - V)$ is dense, and it relates both classes of operators.

Definition 5.1 *An isometric operator is a linear operator V on $\mathcal{H}$ such that $||V\varphi|| = ||\varphi||$ for all $\varphi \in D(V)$.*

Remark 5.2 *Isometric operators also preserve the inner product due to the polarization*

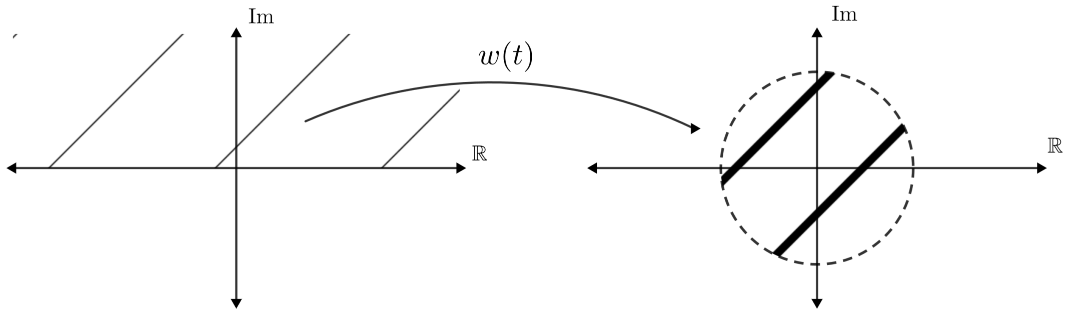

Figure 5.2. $w(t)$ sends the upper half-plane into unit disk

identity, i.e.,

$$\langle V\varphi, V\psi\rangle = \langle \varphi, \psi\rangle \ , \tag{5.5}$$

where polarization identity (Kreyszig, 1978) is given by:

$$\langle V\varphi, V\psi\rangle = \frac{1}{4}\left[||V(\varphi+\psi)||^2 - ||V(\varphi-\psi)||^2 + i||V(\varphi-i\psi)||^2 - i||V(\varphi+i\psi)||^2\right] \ . \tag{5.6}$$

This implies that if V preserves the norm, it also preserves the inner product.

Let us give some properties of isometric operators.

Proposition 5.3 *Let V be an isometric operator. Then,*

(i) V^{-1} exists and isometric.

(ii) V is closed iff $D(V)$ is a closed linear subspace of $\mathcal{H}$.

Proof: (i) First of all, we need to show V^{-1} exists. Suppose $V\varphi = 0$. Then

$$||\varphi|| = ||V\varphi|| = 0 \ , \tag{5.7}$$

implies $\varphi = 0$.

Let $V\varphi = \psi$, then $\varphi = V^{-1}\psi$. This implies

$$||\psi|| = ||V\varphi|| = ||\varphi|| = ||V^{-1}\psi|| \ . \tag{5.8}$$

That is V^{-1} is also isometric.

(ii) Suppose $D(V)$ is closed. Let $(\varphi_m, V\varphi_m) \to (\varphi, \psi)$. Then, $\varphi \in D(V)$ since $D(V)$ is closed. Then

$$\begin{aligned} ||V\varphi - \psi|| &= ||V\varphi - V\varphi_m + V\varphi_m - \psi|| && (5.9)\\ &\leq ||V\varphi - V\varphi_m|| + ||V\varphi_m - \psi|| && (5.10)\\ &= ||V(\varphi - \varphi_m)|| + ||V\varphi_m - \psi|| \ , && (5.11) \end{aligned}$$

where we have used the triangle inequality and the linearity of V. Using isometry of V, we get

$$||V\varphi - \psi|| \leq ||\varphi - \varphi_m|| + ||V\varphi_m - \psi|| \ . \tag{5.12}$$

Since $\{V\varphi_m\}_{m=1}^{\infty}$ goes to ψ and $\{\varphi_m\}_{m=1}^{\infty}$ goes to φ as $m \to \infty$, $V\varphi = \psi$. This proves that V is closed, due to the positive definiteness of the norm.

The proof of other part follows immediately from the definition of closed operator (it has a closed graph $\Gamma(V)$) (see for instance (Schmüdgen, 2012)). □

We have also further properties of isometric operators. Let V be an isometric operator on $\mathcal{H}$. From the inequality

$$||(V - zI)\varphi|| \geq |\ ||V\varphi - |z|||\varphi||\ | = |(1 - z)|\ ||\varphi|| \ , \tag{5.13}$$

for any $\varphi \in D(V)$ and $z \in \mathbb{C}$, it follows that $\mathbb{C} \backslash C \subseteq \pi(V)$. Hence, we can define the deficiency indices for isometric operator by Proposition 4.9:

Definition 5.4 *The following dimensions of the vector spaces*

$$d^i(V) := d_z(V) = dim\left[Ran(V - zI)^{\perp}\right] \text{ for } |z| < 1 \ , \tag{5.14}$$

$$d^e(V) := d_z(V) = dim\left[Ran(V - zI)^{\perp}\right] \text{ for } |z| > 1 \tag{5.15}$$

are called the deficiency indices of the isometric operator V.

As we have seen that $d^i(V)$ and $d^e(V)$ are independent of z. This suggests us to express them purely independent of z:

Lemma 5.5 *If* V *is isometric, then the deficiency indices are simplified to*

$$d^i(V) = dim\left[Ran(V)^{\perp}\right] \ , \tag{5.16}$$

$$d^e(V) = dim\left[D(V)^{\perp}\right] \ . \tag{5.17}$$

Proof: From Equation (5.14), we have

$$d^i(V) = d_0(V) = dim\left[Ran(V)^{\perp}\right] \ . \tag{5.18}$$

For the proof of second equation we fix $z \in \mathbb{C}$, $0 < |z| < 1$. Since $(V^{-1} - z)V\varphi = (I - zV)\varphi = -z(v - z^{-1})\varphi$ for $\varphi \in D(V)$, we obtain $Ran(V^{-1} - zI) = Ran(V - z^{-1}I)$ and therefore by Equation (5.15),

$$\begin{aligned} d^e(V) &= dim\left[Ran(V - z^{-1}I)^{\perp}\right] = dim\left[Ran(V^{-1} - zI)^{\perp}\right] \\ &= d^i(V^{-1}) = dim\left[Ran(V^{-1})^{\perp}\right] = dim\left[D(V)^{\perp}\right] \ . \end{aligned}$$

See for instance (Schmüdgen, 2012). □

Lemma 5.6 *Let* V *be an isometric operator on* $\mathcal{H}$ *and* $\overline{Ran(I - V)} = \mathcal{H}$. *Then,* $Ker(I - V) = \{0\}$.

Proof: Let $\varphi \in Ker(I - V)$. For $\psi \in D(V)$, we have

$$\langle (I - V)\psi, \varphi \rangle = \langle \psi, \varphi \rangle - \langle V\psi, \varphi \rangle \ . \tag{5.19}$$

Since $\varphi \in Ker(I - V)$, we have $(I - V)\varphi = 0$, i.e., $V\varphi = \varphi$. Then

$$\langle (I - V)\psi, \varphi \rangle = \langle \psi, \varphi \rangle - \langle V\psi, V\varphi \rangle = \langle \psi, \varphi \rangle - \langle \psi, \varphi \rangle = 0 \ . \tag{5.20}$$

That is $\varphi = 0$ since $Ran(I - V)$ is dense (see for instance (Schmüdgen, 2012)). □

Now, we are going to construct an isometric operator from a given symmetric operator:

Let T be a (densely defined) symmetric operator on $\mathcal{H}$. If $\mathrm{Im}(z) > 0$, we have $\overline{z} \in \pi(T)$ by the Lemma 4.3. Hence, thanks to the Proposition 4.6 (i), $T - \overline{z}I$ has a bounded inverse which is defined on $Ran(T - \overline{z}I)$. Then we define the following operator

$$V_T := (T - zI)(T - \bar{z}I)^{-1} \ , \tag{5.21}$$

which is called the Cayley transform of T. In other words, $V_T : Ran(T - \overline{z}I) \to Ran(T - zI)$, and

$$V_T(T - \overline{z}I)\varphi = (T - zI)\varphi \ , \tag{5.22}$$

where $\varphi \in D(T)$. So $D(V_T) = Ran(T - \overline{z}I)$ or

$$V_T\psi = (T - zI)\varphi \ , \tag{5.23}$$

where $\psi \in D(V_T)$ and $\varphi \in D(T)$, and $\psi = (T - \overline{z}I)\varphi$.

5.2. Some Propoerties of Cayley Transform

Proposition 5.7 *(i) The Cayley Transform V_T is an isometric operator on $\mathcal{H}$ and its domain and range are given by $D(V_T) = Ran(T - \overline{z}I)$, $Ran(V_T) = Ran(T - zI)$, respectively.*

(ii) $Ran(I - V_T) = D(T)$, $T = (zI - \overline{z}V_T)(I - V_T)^{-1}$ (Since $D(T)$ is assumed to be dense in $\mathcal{H}$, so is $Ran(T - V_T)$).

(iii) T is closed operator iff V_T is closed operator.

(iv) Let S be a symmetric operator on $\mathcal{H}$. Then, $T \subseteq S$ iff $V_T \subseteq V_S$.

(v) The deficiency indices of the symmetric operator is expressed with the deficiency indices of its Cayley transform, that is, $d^i(V_T) = d_-(T)$, and $d^e(V_T) = d_+(T)$.

Proof: (i)Let $z = \lambda + i\mu$. Then, Equation (3.42) implies

$$||(T - zI)\varphi||^2 = ||(T - \lambda I)\varphi||^2 + |\mu|\ ||\varphi||^2 = ||(T - \overline{z}I)\varphi||^2 \ , \tag{5.24}$$

where $\varphi \in D(T)$. Defining $\psi := (T - \overline{z}I)\varphi$, we have

$$V_T\psi = V_T(T - \overline{z}I)\varphi = (T - zI)\varphi \ , \tag{5.25}$$

where $\varphi \in D(T)$. Therefore,

$$||V_T\psi|| = ||(T - zI)\varphi|| = ||(T - \overline{z}I)\varphi|| = ||\psi|| \ , \tag{5.26}$$

that is V_T is isometric and the Equation (5.22) yields to the result that $Ran(V_T) = Ran(T - zI)$.

(ii) Recall $z - \overline{z} \neq 0$ when $\mathrm{Im}(z) > 0$. Since

$$(I - V_T)\psi = (T - \overline{z}I)\varphi - (T - zI)\varphi = (z - \overline{z})\varphi \ , \tag{5.27}$$

$Ran(I - V_T) = D(T)$ is dense. By Lemma 5.6, $Ker(I - V_T) = \{0\}$, so $(I - V_T)^{-1}$ exists.

Then, from the equations

$$(I - V_T)\psi = (z - \overline{z})\varphi \ , \tag{5.28}$$

and

$$\begin{aligned}
(zI - \overline{z}V_T)\psi = z\psi - \overline{z}(T - zI)\varphi &= z\psi - \overline{z}T\varphi + z\overline{z}\varphi && (5.29)\\
&= z(T - \overline{z}I)\varphi - \overline{z}T\varphi + z\overline{z}\varphi && (5.30)\\
&= zT\varphi - z\overline{z}\varphi - \overline{z}T\varphi + z\overline{z}\varphi && (5.31)\\
&= (z - \overline{z})T\varphi \ , && (5.32)
\end{aligned}$$

we get $(zI - \overline{z}V_T)\psi = (z - \overline{z})T\varphi$. Then, it follows that

$$\begin{aligned}
(zI - \overline{z}V_T)\psi &= (z - \overline{z})T\varphi && (5.33)\\
(zI - \overline{z}V_T)(I - V_T)^{-1}(z - \overline{z})\varphi &= (z - \overline{z})T\varphi \ . && (5.34)
\end{aligned}$$

That is

$$T\varphi = (zI - \overline{z}V_T)(I - V_T)^{-1}\varphi \ , \tag{5.35}$$

for $\varphi \in D(T)$. If $\varphi \in D((zI - \overline{z}V_T)(I - V_T)^{-1})$, then we expect in particular (composition of operators) $\varphi \in D((I - V_T)^{-1}) = Ran(I - V_T) = D(T)$. So we have proved

$$T = (zI - \overline{z}V_T)(I - V_T)^{-1} \ . \tag{5.36}$$

(iii) Since T is closed, $Ran(T - \overline{z}I)$ is closed by Proposition 4.6 (iv). By the definition of V_T, we have $D(V_T) = Ran(T - \overline{z}I)$. Then $D(V_T)$ is closed. Thanks to the Proposition 5.3, V_T is closed.

Conversely, let V_T is closed. Then $D(V_T)$ is a closed subspace of $\mathcal{H}$, or $Ran(T -$

$\overline{z}I) = D(V_T)$ is a closed subspace of $\mathcal{H}$. Therefore, if we have $\varphi_m \to \varphi$ and $T\varphi_m \to \psi$, we have $(T - \overline{z}I)\varphi_m \to \psi - \overline{z}\varphi \in Ran(T - \overline{z}I)$. Then, there exists a $\varphi' \in D(T)$ such that

$$(T - \overline{z}I)\varphi' = \psi - \overline{z}\varphi \tag{5.37}$$

or

$$(T - \overline{z}I)(\varphi_m - \varphi') \to 0 \ , \tag{5.38}$$

as $m \to \infty$ in $\mathcal{H}$. Since T is symmetric, the Equation 3.42 implies that $Ker(T - \overline{z}I) = \{0\}$. Hence $\varphi_m \to \varphi' = \varphi$, that is $\varphi \in D(T)$ and $T\varphi = \psi$.

(iv) From Equation (5.22) it immediately follows that S is an extension of T if and only if V_S is an extension of V_T.

(v) Using Lemma 5.5 and Proposition 5.7 (i), we have

$$d^i(V_T) = dim[Ran(V_T)^\perp] = dim[Ran(T - zI)^\perp] = d_-(T) \ , \tag{5.39}$$

and

$$d^e(V_T) = dim[D(V_T)^\perp] = dim[Ran(T - \overline{z}I)^\perp] = d_+(T) \ . \tag{5.40}$$

See for instance (Schmüdgen, 2012). □

Now, we will proceed in the reverse direction and suppose that V is any isometric operator on $\mathcal{H}$ such that $Ran(I - V)$ is dense. Then, by Lemma 5.6, $(I - V)^{-1}$ exists. Then, analogous to the inverse Möbius transformation we can define the operator

$$T_V := (zI - \overline{z}V)(I - V)^{-1} \ , \tag{5.41}$$

with domain $D(T_V) = Ran(I - V)$. This operator is called the inverse Cayley Transform of V(V is the Cayley Transform of T). By this definition, we have

$$T_V(I - V)\varphi = (zI - \overline{z}V)\varphi \ , \tag{5.42}$$

for $\varphi \in D(V)$.

Proposition 5.8 *The above defined operator T_V in Equation (5.41) is a symmetric operator whose Cayley Transform is V.*

Proof: Let $\varphi \in D(T_V)$, then $\varphi = (I - V)\psi$ for some $\psi \in D(V)$ ($D(T_V) = Ran(I - V)$).

Using the assumption that V is isometric and Equation (5.42), we have

$$\begin{aligned}
\langle T_V\varphi, \varphi\rangle &= \langle T_V(I - V)\psi, (I - V)\psi\rangle \\
&= \langle (zI - \overline{z}V)\psi, (I - V)\psi\rangle \\
&= \overline{z}||\psi||^2 + z||V\psi||^2 - \overline{z}\langle\psi, V\psi\rangle - z\langle V\psi, \psi\rangle \\
&= (\overline{z} + z)||\psi||^2 - 2\,\mathrm{Re}[z\langle V\psi, \psi\rangle] \\
&= 2\,\mathrm{Re}(z)||\psi||^2 - 2\,\mathrm{Re}[z\langle V\psi, \psi\rangle] \ .
\end{aligned}$$

Hence $\langle T_V\varphi, \varphi\rangle$ is real, that is

$$\langle T_V\varphi, \varphi\rangle = \overline{\langle T_V\varphi, \varphi\rangle} = \langle \varphi, T_V\varphi\rangle \ ,$$

for all $\varphi \in D(T_V)$. It remains to show that $D(T_V)$ is dense in $\mathcal{H}$. Indeed, since $D(T_V) = Ran(I - V)$ is dense in, T_V is symmetric.

Next, we need to show that V is the Cayley Transform of T_V. Using definition of T_V, and Equation (5.42), we have

$$(T_V - \overline{z})(I - V)\varphi = T_V(I - V)\varphi - \overline{z}(I - V)\varphi = (zI - \overline{z}V)\varphi - \overline{z}(I - V)\varphi = (z - \overline{z})\varphi \ .$$

Since T_V is symmetric (and $z \in \pi(T_V)$), $Ker(T_V) = \{0\}$, $T_V - zI$ (and $T_V - \overline{z}I$) has inverse. So we are allowed to rewrite the above equation as follows:

$$(I - V)\varphi = (T_V - \overline{z}I)^{-1}(z - \overline{z})\varphi \ . \tag{5.43}$$

Similarly, we find

$$(T_V - zI)(I - V)\varphi = (z - \overline{z})V\varphi \ . \tag{5.44}$$

Plugging Equation (5.43) into Equation (5.44), we get

$$(T_V - zI)(T_V - \overline{z}I)^{-1}(z - \overline{z})\varphi = (z - \overline{z})V\varphi \ . \tag{5.45}$$

Therefore $V\varphi = (T_V - zI)(T_V - \overline{z}I)^{-1}\varphi$ for all $\varphi \in D(V)$. Thus, we have shown that $V \subseteq (T_V - zI)(T_V - \overline{z}I)^{-1}$ ($D(V) \subseteq D\left((T_V - zI)(T_V - \overline{z}I)^{-1}\right)$).

For well-definedness of the composition of operators $D(AB) = \{\varphi \in D(B) : B\varphi \in D(A)\} \subseteq D(B)$. So we have

$$D((T_V - zI)(T_V - \overline{z}I)^{-1}) \subseteq D((T_V - \overline{z}I)^{-1}) = Ran(T_V - \overline{z}I) = D(V) \ . \tag{5.46}$$

Hence $D(V) = D((T_V - zI)(T_V - \overline{z}I)^{-1})$ and their actions are the same, that is, $V\varphi = ((T_V - zI)(T_V - \overline{z}I)^{-1}\varphi$ for all $\varphi \in D(V)$. V is the Cayley Transform of T_V. □

Collecting the statements (i) and (ii) of Proposition 5.7, we now have the following theorem ((Schmüdgen, 2012)):

Theorem 5.9 *The Cayley Transform*

$$T \longmapsto V_T = (T - zI)(T - \overline{z}I)^{-1} \tag{5.47}$$

is a bijective mapping from the set of symmetric operators onto the set of all isometric operator V such that $Ran(I - V)$ is dense in $\mathcal{H}$. Its inverse is given by the inverse Cayley Transform formula:

$$V \longmapsto T_V = (zI - \overline{z}V)(I - V)^{-1} \ . \tag{5.48}$$

There are several simple consequences of the above theorem:

Corollary 5.10 *A symmetric operator T is self-adjoint iff Cayley Transform V_T of T is unitary.*

Proof: Thanks to the Basic Criteria for self-adjointness (Theorem 4.20), the symmetric operator T is self-adjoint if and onyl if

$$Ran(T - zI) = \mathcal{H} \ , \tag{5.49}$$

and

$$Ran(T - \overline{z}I) = \mathcal{H} \ , \tag{5.50}$$

where $\mathrm{Im}(z) > 0$. Since $D(V_T) = Ran(T - \overline{z}I)$ and $Ran(V_T) = Ran(T - zI)$, the conditions (5.49) and (5.50) hold if and only if the isometric operator V_T is unitary, i.e., $D(V_T) = \mathcal{H}$ and $Ram(V_T) = \mathcal{H}$ (see for instance (Schmüdgen, 2012)). □

Corollary 5.11 *A unitary operator V is the Cayley transform of a self-adjoint operator iff the kernel of $I - V$ satisfies $Ker(I - V) = \{0\}$.*

Proof: Theorem 5.9 and Corollary 5.10 implies that V is the Cayley Transform of a self-adjoint operator if and only if $Ran(I - V)$ is dense, that is

$$Ran(I - V)^{\perp} = \{0\} = Ker((I - V)^{*}) = Ker(I - V^{*}) \ ,$$

since I and V are bounded operators. So

$$Ker(I - V^{*}) = \{0\} \ .$$

Indeed this is equivalent to $Ker(I - V) = \{0\}$ since V is unitary. To show this we suppose $Ker(I - V) = \{0\}$, that is, $(I - V)\varphi = 0$, implies $\varphi = 0$. We may rewrite the first equation as follows:

$$\varphi = V\varphi \ , \tag{5.51}$$

and since V is unitary operator, multiplying Equation (5.51) by V^* from the left we get

$$V^*\varphi = \underbrace{V^*V}_{I}\varphi = \varphi \ . \tag{5.52}$$

This means that $(V^* - I)\varphi = 0$ implies $\varphi = 0$, that is $Ker(V^* - I) = \{0\}$.

Conversely, we suppose $Ker(V^* - I) = \{0\}$. Instead of Equation (5.51) we have

$$\varphi = V^*\varphi \ , \tag{5.53}$$

and we multiply Equation (5.53) by V from the left. Then we get the result that

$$V\varphi = VV^*\varphi = I \tag{5.54}$$

implies $\varphi = 0$. That is $Ker(V - I) = \{0\}$ (see for instance (Schmüdgen, 2012)). $\square$

Corollary 5.12 *Let T be a symmetric operator on $\mathcal{H}$. If $d_+(T)$ or $d_-(T)$ is finite, then each symmetric extension S of the closure of T is closed.*

Proof: Suppose $d_+(T)$ is finite (otherwise, we replace T by $-T$ and use the relation $d_\pm(T) = d_\mp(-T)$). From Proposition 5.7 (iv), the Cayley Transform V_S of a symmetric extension S of $\overline{T}$ is an extension of $V_{\overline{T}}$, that is $V_{\overline{T}} \subseteq V_S$. Since $\overline{T}$ is closed, V_T is closed thanks to Propositon 5.7 (iii). Therefore $D(V_{\overline{T}})$ is closed. Then, Theorem 3.5 implies

$$\begin{aligned} \mathcal{H} &= D(V_{\overline{T}}) \oplus D(V_{\overline{T}})^\perp \\ &= D(V_{\overline{T}}) \oplus Ran(\overline{T} - zI)^\perp \\ &= D(V_{\overline{T}}) \oplus Ker(\overline{T}^* - zI) \\ &= D(V_{\overline{T}}) \oplus Ker(T^* - zI) \ . \end{aligned}$$

Defining $N_z = Ker(T^* - zI)$, we rewrite the last step as follow:

$$\mathcal{H} = D(V_{\overline{T}}) \oplus Ker(T^* - zI) \ . \tag{5.55}$$

Using $D(V_{\overline{T}}) \subseteq D(V_S)$, and the decomposition (5.55) of $\mathcal{H}$, there is a linear subspace ϵ of N_z such that

$$D(V_S) = D(V_{\overline{T}}) \oplus \epsilon \ . \tag{5.56}$$

Since $d_+(T) = dim(N_z)$ is finite, ϵ should be also finite dimensional. Hence $D(V_S)$ is also closed thanks to Equation (5.56).

Hence, S is closed by Proposition 5.7 (iii) (see for instance (Schmüdgen, 2012)). □

Remark 5.13 *The Cayley Transform V_T defined above depends on z from the upper half-plane. In applications, it is often convenient to take $z = i$. Let us restate the corresponding formulas in the special case $z = i$. Therefore*

$$V_T := (T - i)(T + i)^{-1} \ , \tag{5.57}$$

where $D(V_T) = Ran(T + i)$ and $Ran(V_T) = Ran(T - i)$, and we define

$$T_V := i(I + V_T)(I - V_T)^{-1} \ , \tag{5.58}$$

where $D(T_V) = Ran(I - V_T)$ and $Ran(T_V) = Ran(I + V_T)$.

5.3. Von Neumann's Extension Theory of Symmetric Operators

While we are speaking of a symmetric (respectively self-adjoint) extension of T, we mean a symmetric (respectively self-adjoint) operator S acting on the same Hilbert space $\mathcal{H}$ such that $T \subseteq S$.

Proposition 5.14 *Let T be a symmetric operator and S be a self-adjoint operator. Then $T \subseteq S$ if and only if $S \subseteq T^*$.*

Proof: Suppose $T \subseteq S$, then Proposition 3.39 (i) implies that $S^* \subseteq T^*$. Since S is self-adjoint, we get $S \subseteq T^*$.

Conversely, suppose $S \subseteq T^*$, Proposition 3.39 (i) implies that $T^{**} \subseteq S^*$. Since S is self-adjoint we get $T^{**} \subseteq S$. Since $T^{**} = \overline{T}$ is the smallest closed extension, we get $T \subseteq \overline{T} \subseteq S$. That is $T \subseteq S$. □

Above Proposition tells us that any self-adjoint extension S of T is completely described by its domain $D(S)$, since

$$S = T^*|_{D(S)} \ . \tag{5.59}$$

The Cayley Transform allows us to reduce the (difficult) problem of describing all symmetric extensions of T to the (easier) problem of finding all isometric extensions of the Cayley Transform V_T.

From Proposition 5.7 (iv), if S is a symmetric extension of T, then V_S is an isometric extension of V_T.

Conversely, let V be an isometric operator on $\mathcal{H}$ such that $V_T \subseteq V$.

Let us show that $Ran(I - V_T) \subseteq Ram(I - V)$. For this, let $\psi \in Ran(I - V_T)$. Then there exists $\varphi \in D(I - V_T)$ such that $(I - V_T)\varphi = \psi$, i.e.,

$$\varphi - V_T\varphi = \psi \ .$$

Since $V_T \subseteq V$, that is, $V_T\varphi = V\varphi$ for any $\varphi \in D(V_T)$. So above equation becomes

$$\varphi - V\varphi = \psi \ ,$$

or $(I - V)\varphi = \psi$. That is $\psi \in Ran(I - V)$. Then $Ran(I - V_T) \subseteq Ran(I - V)$. Therefore $\overline{Ran(I - V_T)} = \mathcal{H}$ implies $\overline{Ran(I - V)} = \mathcal{H}$. Hence, V is the Cayley Transform of a symmetric operator S and $T \subseteq S$.

This procedure leads us to a parametrization of all closed symmetric extensions because of the Proposition 5.7 (iii).

Theorem 5.15 (Structure of Isometric Extensions) *Let F and G be two closed subspaces of $\mathcal{H}$ and*

$$V : F \longrightarrow G \ ,$$

be an isometry. Let $F_+ \subseteq F^\perp$ and $F_- \subseteq G^\perp$ be closed subspaces. Then,

$$V' : F \oplus F_+ \longrightarrow G \oplus F_- \ ,$$

is an isometric extension of V iff $dim F_+ = dim F_-$ and there exists an isometry

$$U : F_+ \longrightarrow F_- \ ,$$

so that for any $f \in F \oplus F_+$, i.e., $f = f_0 + f_+$, where $f_0 \in F$, $f_+ \in F_+$ and

$$V'f := V f_0 + U f_+ \ . \tag{5.60}$$

Proof: ($\Longleftarrow$) First we show V' is an isometry. Since V is onto G and U is onto F_-, V' is onto $G \oplus F_-$. To show the norm is preserved we take $f \in F \oplus F_-$ and use the definition of V', then we get

$$\begin{aligned} ||V'f||^2 = \langle V'f, V'f \rangle &= \langle V f_0 + U f_+, V f_0 + U f_+ \rangle \\ &= \langle V f_0, V f_0 \rangle + \langle V f_0, U f_+ \rangle + \langle U f_+, V f_0 \rangle + \langle U f_+, U f_+ \rangle \ . \end{aligned}$$

Since $V f_0 \in G$ and $U f_+ \in F_-$, and $F_- \subseteq G^\perp$, we get

$$||V'f||^2 = ||V f_0||^2 + ||U f_+||^2 = ||f_0||^2 + ||f_+||^2 = ||f||^2 \ ,$$

where we have used the fact that operators U and V are isometry.

Since $F = D(V) \subseteq D(V') = F \oplus F_+$ and for any $f \in F = D(V)$

$$V'f = Vf \ ,$$

the operator V' is an extension of V. Hence V' is an isometric extension of V.

($\Longrightarrow$) Now suppose that V' is an isometry such that $V \subseteq V'$. Let $f_+ \in F_+$ and we define

$$Uf_+ := V'f_+ \ . \tag{5.61}$$

Since V is symmetric and onto G, for any $g \in G$ there exists $f \in F$ such that $Vf = g$. Therefore,

$$\langle g, Uf_+\rangle = \langle Vf, Uf_+\rangle = \langle V'f, V'f_+\rangle = \langle f, f_+\rangle = 0 \ .$$

This means that $g = Uf_+ \perp G$ and hence U maps F_+ into F_-, and U preserves the norm since V' does.

We now have to show that U is onto. For any $f_- \in F_-$ there exists $f \in F \oplus F_+$ so that $V'f = f_-$ because V' is onto. For any $f_0 \in F$ we have

$$0 = \langle Vf_0, V'f\rangle = \langle V'f_0, V'f\rangle = \langle f_0, f\rangle \ .$$

Hence $f \in F_+$ and $V'f = Uf = f_-$ and we get $V'f = Vf_0 + Uf_-$ (see for instance (Weidmann, 2012)). $\square$

Theorem 5.16 (Closed Symmetric Extension) *Let T be a symmetric operator on $\mathcal{H}$. Suppose that $F_+ \subseteq Ker(T^* - zI) = Ran(T - \overline{z}I)^\perp = D(V_T)^\perp$ and $F_- \subseteq Ker(T^* - \overline{z}I) = Ran(T - zI)^\perp = Ran(V_T)^\perp$ are closed linear subspaces of $\mathcal{H}$ such that $dimF_+ = dimF_-$. Furthermore, suppose that U is an isometric linear mapping of F_+ onto F_-. If we define*

$$D(T_U) := D(\overline{T}) \dotplus (I - U)F_+ \ , \tag{5.62}$$

and $T_U = T|^*_{D(T_U)}$, i.e., $T_U(\varphi + (I - U)\psi) = \overline{T}\varphi + z\psi - \overline{z}U\psi$ for $\varphi \in D(\overline{T})$ and $\psi \in$

F_+, then, T_U is a closed symmetric extension of T. Furthermore, any closed symmetric extension of T on $\mathcal{H}$ is of this form and

$$d_\pm(T) = d_\pm(T_U) + dimF_\pm \ .$$

Proof: Since any closed extension of T is an extension of $\overline{T}$ ($\overline{T}$ is the smallest closed extension of T) and $\overline{T}^* = T^*$ (thanks to Theorem 3.49 (iii)), we can assume that T is closed without loss of generality. In some sense, we are looking for the nontrivial closed extensions of T: $T \subseteq \overline{T} \subseteq T_U \subseteq T^*$. Then by Proposition 5.7, $D(V_T)$ is closed and closed symmetric extensions of T are in one-to-one correspondence with isometric extensions V of V_T for which $D(V)$ is closed.

From the previous theorem (Theorem 5.15), we have $D(V) = D(V_T) \oplus F_+$ and $V\psi = V_T\psi$ for $\psi \in D(V_T)$ (Since V is an extension) and $V\psi = U\psi$ for $\psi \in F_+$, where $U, F_\pm$ are defined as in the Theorem 5.15. Because of the one-to-one correspondence between isometric operators and symmetric operators, we define the symmetric operator, from the extended isometric operator V:

$$T_U := (zI - \overline{z}V)(I - V)^{-1} \ .$$

Then Proposition 5.7 implies

$$D(T_U) = Ran(I - V) = (I - V)\xi = (I - V)(D(V_T) \oplus F_+) \ ,$$

where $\xi \in D(V)$. Letting $\dot{+}$ as the direct sum of vector spaces (not need to be orthogonal) and using Proposition 5.7, we get

$$\begin{aligned} D(T_U) &= (I - V)D(V_T) \dot{+} (I - V)F_+ \\ &= (I - V_T)D(V_T) \dot{+} (I - U)F_+ \\ &= D(T) \dot{+} (I - U)F_+ \ . \end{aligned}$$

The three last sums in the proceeding equations are direct, because $(I - V)$ is injective by Lemma 5.6 ($(I - V)(\psi + \varphi) = 0$ implies $\psi + \varphi = 0$, and this also implies $\varphi = 0$ and $\psi = 0$ since $\varphi \perp \psi$). Since $T_U \subseteq T_U^* \subseteq T^*$ and hence

$$T_U(\varphi + (I - U)\psi) = T^*(\varphi + (I - U)\psi) = T^*\varphi + T^*\psi - T^*U\psi = \overline{T}\varphi + z\psi - \overline{z}U\psi \ ,$$

where $\varphi \in D(\overline{T})$ and $\psi \in F_+$. Lemma 5.5 and Proposition 5.7 implies

$$dim D(V)^{\perp} = d^e(V) = d_+(T_U) \ ,$$

and

$$dim D(V_T)^{\perp} = d^e(V_T) = d_+(T) \ .$$

Since $D(V) = D(V_T) \oplus F_+$, we have $D(V_T)^{\perp} = D(V) \oplus F_+$. This can be shown as follows: Since $D(V)$ is closed it is a Hilbert space. According to Hilbert space decomposition and $D(V_T) \oplus F_+ = D(V) \subseteq \mathcal{H}$, we must have $F_+ \subseteq D(V_T)^{\perp}$ and $D(V_T) \subseteq F_+^{\perp}$. Moreover, $D(V_T) \subseteq D(V)$ and $F_+ \subseteq D(V)$. This implies that $D(V)^{\perp} \subseteq D(V_T)^{\perp}$ and $D(V)^{\perp} \subseteq F_+^{\perp}$. Since $D(V_T)^{\perp}$ is closed and

$$D(V)^{\perp} \oplus X = D(V_T)^{\perp} \subseteq \mathcal{H} \ ,$$

where $X \subseteq D(V)^{\perp\perp} = \overline{D(V)} = D(V)$. There could be 2 options: either $X = D(V_T)$, or $X = F_+$. If we had $X = D(V_T)$, we would get $D(V_T)^{\perp} = \mathcal{H}$. Hence we should have $X = F_+$, so $D(V_T)^{\perp} = D(V)^{\perp} \oplus F_+$.

This result implies that

$$d_+(T) = d_+(T_U) + dim F_+ \ . \tag{5.63}$$

Similarly,

$$d_-(T) = d_-(T_U) + dim F_- \ . \tag{5.64}$$

See for instance (Schmüdgen, 2012)). □

Theorem 5.17 (Von Neumann's Theorem on Self-adjoint Extension) *Let T be a symmetric operator. Then, T has self-adjoint extension iff the deficiency indices coincide:*

$$d_+(T) = d_-(T) \ . \tag{5.65}$$

If $d_+(T) = d_-(T)$, then all self-adjoint extension of T are given by the operators T_U where U is an isometric mapping from $Ker(T^* - zI)$ onto $Ker(T^* - \overline{z}I)$ such that

$$T_U(\varphi + (I - U)\psi) := \overline{T}\varphi + z\psi - \overline{z}U\psi \ , \tag{5.66}$$

where

$$D(T_U) = D(\overline{T}) \dot{+} (I - U)Ker(T^* - zI) \tag{5.67}$$

for $\varphi \in D(\overline{T})$ and $\psi \in Ker(T^* - zI)$.

Proof: Corollary 5.10 implies that an operator T_U from Theorem 5.16 is self-adjoint if and only if its Cayley Transform is unitary, or equivalently, if

$$F_+ = Ker(T^* - zI) \ ,$$

and

$$F_- = Ker(T^* - \overline{z}I)$$

in Theorem 5.16. Hence, the description of all self-adjoint extensions of T stated above follows from Theorem 5.16. Clearly, an isometric operator from a closed subspace $\mathcal{H}_1$ onto another closed subspace of $\mathcal{H}_2$ exists if and only if $dim\mathcal{H}_1 = dim\mathcal{H}_2$. Hence, T has a self-adjoint extension on $\mathcal{H}$ that is, there exists an isometric map of $Ker(T^* - zI)$ onto $Ker(T^* - \overline{z}I)$ if and only if $d_+(T) = dimKer(T^* - z) = dimKer(T^* - \overline{z}) = d_-(T)$ (see for instance (Schmüdgen, 2012)). □

Let us summarize the result with the following Figure 5.3.

According to the above theorem, we have three cases:

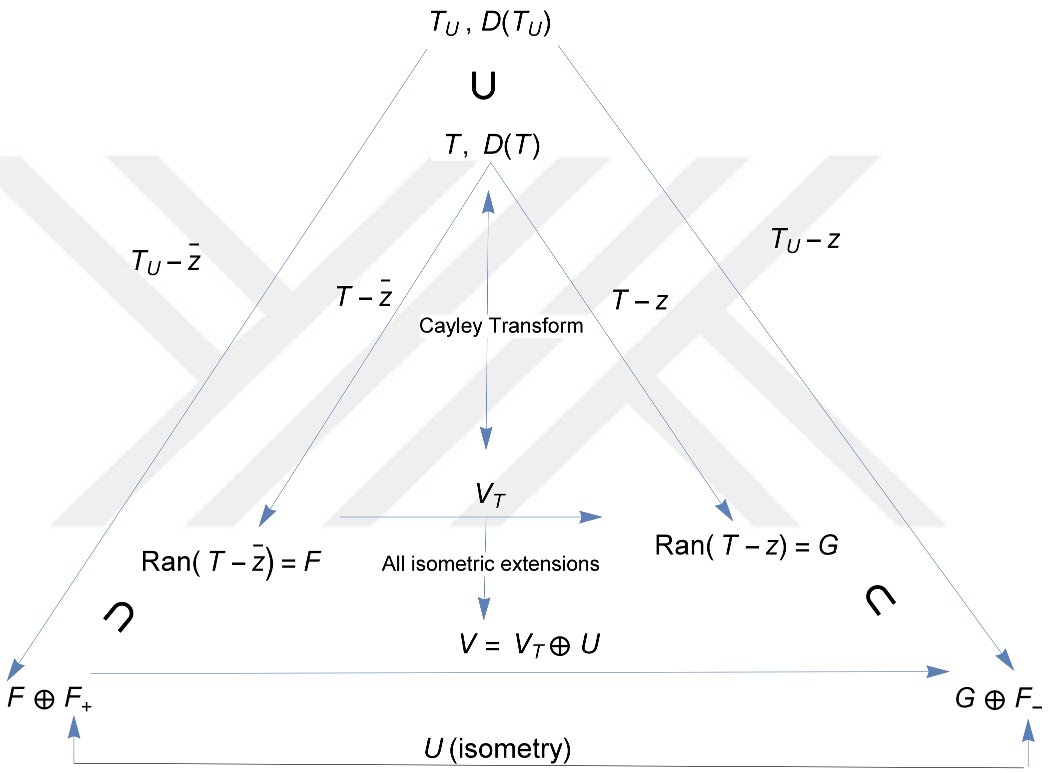

Figure 5.3. Diagram summarizing the construction of the closed symmetric extensions of a symmetric operator. Here $F_+ \subseteq F^\perp$ and $F_- \subseteq G^\perp$.

Case 1 ($d_+(T) = d_-(T) = 0$): In this case $\overline{T}$ is the unique self-adjoint extension of T on $\mathcal{H}$, so T is essentially self-adjoint.

Case 2 ($d_+(T) = d_-(T) \neq 0$): Then, there are infinitely many isometric mappings of $Ker(T^* - zI)$ onto $Ker(T^* - \overline{z}I)$ and have infinitely many self-adjoint extensions of T on $\mathcal{H}$.

Case 3 ($d_+(T) \neq d_-(T)$): There is no self-adjoint extension of T on $\mathcal{H}$.

5.4. Self-adjoint Extension of the Momentum Operator

Example 5.18 (Momentum Operator on $\mathbb{R}$) *Let us recall that the momentum operator is defined by*

$$P\varphi := -i\varphi' \ ,$$

for all $\varphi \in D(P) = H^1(\mathbb{R})$ (see the definition of $H^1(\mathbb{R})$ given in Appendix B). There are useful different characterization of the Sobolev spaces $H^1(\mathbb{R})$, as emphasized in the same Appendix. One another equivalent formulation of these spaces are expressed by absolutely continuous (AC) functions (Schmüdgen, 2012), that is:

$$H^1(\mathbb{R}) = \{\varphi \in L^2(\mathbb{R}) : \varphi \in AC[a,b] \text{ for } [a,b] \subseteq \mathbb{R} \text{ and } \varphi' \in L^2(\mathbb{R})\} \ . \tag{5.68}$$

Here, a function φ on $[a,b]$ is absolutely continuous if and only if there exists a function $\psi \in L^1(a,b)$ such that for all $x \in [a,b]$

$$\varphi(x) = \varphi(a) + \int_a^x \psi(t) \ dt \ .$$

If $\varphi \in AC[0,1]$, then $\varphi \in C([a,b])$, and φ is almost everywhere differentiable with $\varphi'(x) = \psi(x)$ almost everywhere on $[a,b]$. We simply denote $\varphi' = \psi$. Since for any absolutely continuous functions ψ and φ, we have the integration by parts formula

$$\langle \varphi', \psi \rangle + \langle \varphi, \psi' \rangle = \overline{\varphi(b)}\psi(b) - \overline{\varphi(a)}\psi(a) \ . \tag{5.69}$$

Let us show that if $\varphi \in H^1(\mathbb{R})$, then $\lim_{x\to\pm\infty} \varphi(x) = 0$. For simplicity, we will prove this for $H^1(0,\infty)$. Suppose that $\varphi \in H^1(0,b)$, then according to the integration by parts formula we have

$$\langle \varphi', \varphi\rangle + \langle \varphi, \varphi'\rangle = \overline{\varphi(b)}\varphi(b) - \overline{\varphi(0)}\varphi(0) = |\varphi(b)|^2 - |\varphi(0)|^2 \ , \tag{5.70}$$

for any $b > 0$. By the definition of $H^1(0,\infty)$, we have $\varphi \in L^2(\mathbb{R})$ and $\varphi' \in L^2(\mathbb{R})$. Hence, $\overline{\varphi}\varphi' \in L^1(0,\infty)$ by Cauchy-Schwarz inequality (3.3). Therefore, the left hand side of Equation (5.70) converges as $b \to \infty$. This implies that $\lim_{b\to\infty} |\varphi(b)|^2$ exists. Since $\varphi \in L^2(0,\infty)$, this limit must be zero. This proof can easily be extended to $H^1(\mathbb{R})$.

Let us now show that P is symmetric on this domain $H^1(\mathbb{R})$. For this, we will multiply the integration by parts formula (Equation (5.69)) by i and use the conjugate linearity with respect to the first slot to obtain

$$\langle -i\varphi', \psi\rangle + \langle \varphi, i\psi'\rangle = i[\overline{\varphi(b)}\psi(b) - \overline{\varphi(a)}\psi(a)] \ . \tag{5.71}$$

Taking the limits of both sides as $b \to \infty$ and $a \to -\infty$, we get $\langle -i\varphi', \psi\rangle + \langle \varphi, i\psi'\rangle = 0$, i.e.,

$$\langle P\varphi', \psi\rangle = \langle \varphi, P\psi\rangle \ , \tag{5.72}$$

for all $\varphi, \psi \in H^1(\mathbb{R})$.

To prove that P is self-adjoint on $H^1(\mathbb{R})$, we will use the self-adjoint criteria (Theorem 4.20), that is, we need to show that $Ran(P \pm iI) = \mathcal{H} = L^2(\mathbb{R})$. For this, we will consider the solution of the following equation:

$$(P + iI)\varphi = \chi \ , \tag{5.73}$$

for $\chi \in L^2(\mathbb{R})$. This equation becomes

$$-i\varphi' + i\varphi = \chi \ . \tag{5.74}$$

Taking the Fourier transformation of both sides, we get

$$(p+i)\hat{\varphi}(p) = \hat{\chi}(p) \ . \tag{5.75}$$

Therefore, $\hat{\varphi}(p) = \frac{\hat{\chi}}{p+i}$. This means that for any $\hat{\chi}$ in $L^2(\mathbb{R})$, we can always find a solution $\hat{\varphi}$ in the corresponding domain, i.e., $\int_{\mathbb{R}} |\hat{\varphi}|^2(1+p^2) \ \frac{dp}{(2\pi)} = \int_{\mathbb{R}} |\hat{\chi}|^2 \ \frac{dp}{2\pi} < \infty$. Hence $Ran(P+iI) = \mathcal{H}$. Similarly $Ran(P-iI) = \mathcal{H}$.

Example 5.19 (Momentum Operator on a Bounded Interval) *(Schmüdgen, 2012)*

We consider the momentum operator on some interval where the domain is chosen to be $D(P) = H_0^1(a,b) = \{\varphi \in H^1(a,b) : \varphi(a) = \varphi(b) = 0\}$ and $H^1(a,b) = \{\varphi \in AC[a,b] : \varphi' \in L^2(a,b)\}$. Here $AC[a,b]$ denotes the set of absolutely continuous functions on the interval $[a,b]$. Then, $D(P^*) = H^1(a,b)$ and the action of the adjoint of the momentum operator is

$$P^*\psi = -i\psi' \ ,$$

for all $\psi \in D(P^*)$.

To show this, we first suppose $\psi \in H^1(a,b)$ and $\varphi \in D(P) = H_0^1(a,b)$. Since for any absolutely continuous functions ψ and φ, we have the integration by parts formula

$$\langle \varphi', \psi \rangle + \langle \varphi, \psi' \rangle = \overline{\varphi(b)}\psi(b) - \overline{\varphi(a)}\psi(a) \ .$$

Multiplying both sides by i and using conjugate linearity of inner product with respect to *the first slot we get*

$$\langle -i\varphi', \psi\rangle + \langle \varphi, i\psi'\rangle \;\; = \;\; i[\overline{\varphi(b)}\psi(b) - \overline{\varphi(a)}\psi(a)] \ .$$

Since $\varphi \in D(P) = H_0^1(a,b)$, $\varphi(a) = \varphi(b) = 0$, *we have*

$$\langle -i\varphi', \psi\rangle = -\langle \varphi, i\psi'\rangle = \langle \varphi, -i\psi'\rangle \ . \tag{5.76}$$

Hence

$$\langle \psi, P\varphi\rangle = \langle -i\psi', \varphi\rangle \ .$$

By the definition of adjoint, we obtain $\psi \in D(P^*)$ *and* $P^*\psi = -i\psi'$. *This means* $H^1(a,b) \subseteq D(P^*)$.

Conversely, we suppose $\psi \in D(P^*)$ *and define* $\eta := P^*\psi$ *such that*

$$\xi(x) := \int_a^x \eta(t)\, dt \ .$$

We note that since $\eta \in L^2(a,b) \subseteq L^1(a,b)$, ξ *is well-defined. Moreover,* $\xi(a) = 0$ *and*

$$\xi(x) = \xi(a) + \int_a^x \eta(t)\, dt \ ,$$

and $\xi'(x) = \eta(x)$ *almost everywhere on* $[a,b]$. *Actually, this is a property of absolutely continuous functions, i.e.,*

Hence $\xi \in H^1(a,b)$, *and* $\xi' = \eta$. *Let* $\varphi \in D(P)$, *then*

$$\langle \xi, -\varphi'\rangle = \langle \xi', \varphi\rangle = \langle \eta, \varphi\rangle = \langle P^*\psi, \varphi\rangle = \langle \psi, P\varphi\rangle = \langle \psi, -i\varphi'\rangle \ .$$

We rewrite the left hand side

$$\langle \xi, -\varphi'\rangle = -\langle \xi, \varphi'\rangle = (-i)(-i)\langle \xi, \varphi'\rangle = \langle i\xi, -i\varphi'\rangle \ .$$

Therefore

$$\langle i\xi, -i\varphi\rangle = \langle \psi, -i\varphi'\rangle \ ,$$

which implies

$$\langle \psi - i\xi, -i\varphi'\rangle = 0 \ .$$

or $\psi - i\xi \in Ran(P)^{\perp}$.

Now we will show that $\mathbb{C}^{\perp} \subseteq Ran(P)$ *or equivalently* $Ran(P)^{\perp} \subseteq (\mathbb{C})^{\perp\perp} = \overline{\mathbb{C}} = \mathbb{C}$.

Let $\eta \in (\mathbb{C}.1)^{\perp}$*, and define*

$$\xi(x) := \int_a^x \eta(t)\ dt \ .$$

Since $\eta \in L^2(a,b) \subseteq L^1(a,b)$*, then* $\xi \in H^1(a,b)$ *and* $\xi' = \eta$*. Moreover,* $\xi(a) = 0$ *and* $\xi(b) = \int_a^b \eta(t)dt = \langle 1, \eta\rangle = 0$ *(since* $\eta \in (\mathbb{C}.1)^{\perp}$*). Thus* $\xi \in D(P)$*, and* $P(i\xi) = \eta \in Ran(P)$*.*

Since ξ *and* 1 *belong to* $H^1(a,b)$*, we conclude* $\psi \in H^1(a,b)$ *from the fact that* $Ran(P)^{\perp} \subseteq \mathbb{C}$*. Hence,* $\psi \in D(P^*) \subseteq H^1(a,b)$*. Hence we have shown* $D(P^*) = H^1(a,b)$ *which implies that* P *is not self-adjoint on* $D(P) = H_0^1(a,b)$*.*

Remark 5.20 $D(P)$ *is dense in* $L^2(a,b)$ *(*P *is densely defined, so its adjoint is well defined) and* P *is closed on* $D(P)$*.*

Proof: Since $C_0^{\infty}([a,b])$ is densely defined in $L^2(a,b)$, and $C_0^{\infty} \subseteq H_0^1 \subseteq L^2$, it is immediately seen that $H_0^1(a,b)$ must be also dense in $L^2(a,b)$.

To show P is closed on $D(P)$ we will show $P^{**} = \overline{P} = P$. Since P is symmetric, Corollaries 3.52 and 3.53 implies that $P \subseteq P^{**}$. Therefore it is sufficient to show that $P^{**} \subseteq P$. Let $\varphi \in D(P^{**})$, then Proposition 3.39 (iii) implies that $\varphi \in D(P^*)$ where $D(P^*) = H^1(a,b)$ and $P^{**}\varphi = P^*\varphi = -i\varphi'$ for all $\varphi \in D(P^{**})$. Let $\psi \in D(P^*)$. Using integration by parts formula, we get

$$0 = \langle \varphi, P^*\psi\rangle - \langle P^{**}\varphi, \psi\rangle = \langle \varphi, -i\psi'\rangle - \langle i\varphi', \psi\rangle = i[\psi(b)\overline{\varphi(b)} - \psi(a)\overline{\varphi(a)}] \ .$$

Since the values of $\psi(a)$ and $\psi(b)$ of $\psi \in D(P^*)$ are arbitrary, we conclude that $\varphi(a) = \varphi(b) = 0$. Hence $\varphi \in D(P)$. $\square$

Remark 5.21 *The reason for defining operator P on absolutely continuous functions was to get a closed operator. Often it is more convenient to work with C^∞ functions that vanish at boundaries.*

Proposition 5.22 *Let $D(P_0) := \{\varphi \in C^\infty([a,b]) : \varphi(a) = \varphi(b) = 0\}$ and $P_0\varphi = P\varphi$ for all $\varphi \in D(P_0)$. P_0 is the restriction of P, that is $P_0 = P\big|_{D(P_0)}$. Then, $\overline{P_0} = P$.*

Proof: Our first aim is to show $Ran(P_0)^\perp \subseteq \mathbb{C}.1$. For simplicity, we apply the following liner transformation $x \mapsto \pi(x-a)(b-a)^{-1}$. This maps the interval $[a,b]$ to $[0,\pi]$ so that we can assume $a = 0$ and $b = \pi$ without loss of generality here. Let us take $\sin nx \in D(P_0)$ for $n \in \mathbb{N}$, so $P_0(\sin nx) = -i\cos nx$, or equivalently $\cos nx = in^{-1}P_0(\sin nx) \in Ran(P_0)$. From the theory of Fourier series, we know that the linear span of functions $\cos nx$, $n \in \mathbb{N}_0 = \{0,\ 1,\ \ldots\}$ is dense in $L^2(0,\pi)$ (Rynne and Youngson, 2013). Therefore $\{\cos nx\}_{n\in\mathbb{N}} \subseteq \{\cos nx\}_{n\in\mathbb{N}_0} \subseteq Ran(P_0)$. This implies that

$$Ran(P_0)^\perp \subseteq \{\cos nx\}^\perp_{n\in\mathbb{N}_0} = \{0\} \subseteq \{\cos nx\}^\perp = \mathbb{C}.1\ .$$

By using the same arguments given above, we show that $D(P_0^*) \subseteq H^1(0,\pi)$. Suppose $\psi \in D(P_0^*)$, we set $\eta := P_0^*\psi \in L^2(a,b)$, define $\xi(x) = \int_a^x \eta(t)\ dt$. Then $\xi(a) = 0$ and $\xi'(x) = \eta(x)$ almost everywhere. This implies that $\xi \in H^1(a,b)$. Let $\varphi \in D(P_0)$. Applying integration by parts and almost everywhere derivative of ξ, we get

$$\langle \xi, -\varphi' \rangle = \langle \xi', \varphi \rangle = \langle \eta, \varphi \rangle = \langle P_0^*\psi, \varphi \rangle = \langle \psi, P_0\varphi \rangle = \langle \psi, -i\varphi' \rangle\ .$$

That is

$$\langle \xi, -\varphi' \rangle = \langle \psi, -i\varphi' \rangle\ .$$

Therefore

$$-i^2\langle \xi, -\varphi' \rangle = \langle -i\xi, -i\varphi' \rangle = \langle \xi, -\varphi' \rangle = \langle \psi, -i\varphi' \rangle\ ,$$

which implies that

$$\langle \psi + i\xi, -i\varphi' \rangle = 0\ . \tag{5.77}$$

Then $\psi + i\xi \in Ran(P_0)^{\perp} \subseteq \mathbb{C}.1$. Since ξ and 1 are in $H^1(a,b)$, we conclude that $\psi \in H^1(a,b)$. Hence we have shown that $D(P_0^*) \subseteq H^1(a,b)$. We have chosen $a = 0$ and $b = \pi$, so $D(P_0^*) \subseteq H^1(0,\pi) = D(P^*)$. Therefore $P = \overline{P} = P^{**} \subseteq P_0^{**} = \overline{P_0}$. On the other hand since $\overline{P_0}$ is the smallest closed extension of P_0, $P_0 \subseteq \overline{P_0} \subseteq P$. Hence $\overline{P_0} = P$ (see for instance (Schmüdgen, 2012)). □

Recall that $P\varphi = -i\varphi'$ for $\varphi \in D(P)$ where $D(P) = H_0^1(a,b)$, and $P^*\psi = -i\psi'$ for $\psi \in D(P^*)$ where $D(P^*) = H^1(a,b) = \{\psi \in AC[a,b] : \psi' \in L^2(a,b)\}$.

$\psi \in Ker(P^* - zI)$ if and only if $\psi \in D(P^*)$ and $-i\psi'(x) = z\psi(x)$ on an interval I ($\langle \psi, (P - \bar{z}I)\varphi\rangle = \langle (P^* - zI)\psi, \varphi\rangle = \langle -i\psi' - z\psi, \varphi\rangle = 0$ for all $\varphi \in D(P)$). The equation $-i\psi' = z\psi$ implies that ψ' is also absolutely continuous. Since $AC \subseteq C$, ψ' must be continuous. By repeating this argument, we see that any solution of $P^*\psi = -i\psi' = z\psi$ is infinitely differentiable. For simplicity, we shall choose $z = i$ and $z = -i$, i.e., we are going to find the dimensions of the following closed subspaces:

$$N_{+i} := Ker(P^* - i) \ ,$$

and

$$N_{-i} := Ker(P^* + i) \ .$$

For the dimension of N_{+i}, suppose $(P^* - i)\psi_+ = -i\psi_+' - i\psi_+ = 0$ that yields to the differential equation,

$$\psi_+' + \psi_+ = 0 \ ,$$

whose general solution is $\psi_+ = ce^{-x} \in L^2(a,b)$. Therefore $N_+ = \{ce^{-x} : c \in \mathbb{C}\}$.

For N_- by the same way we suppose $(P^* + i)\psi = -i\psi_+' + i\psi = 0$. Therefore we have the differential equation

$$\psi_-' - \psi_- = 0 \ ,$$

which has the general solution $\psi_- = ce^{x} \in L^2(a,b)$. Therefore $N_- = \{ce^{x} : c \in \mathbb{C}\}$. Hence N_+ and N_- are vector spaces with their bases $\{e^{-x}\}$ and $\{e^{-x}\}$ respectively. So their dimensions are 1. For self-adjoint extensions $F_+ = N_+$ and $F_- = N_-$. We normalize the solutions, for this reason let us choose $a = 0$ and $b = 1$ for simplicity, then suppose

$$\int_0^1 |\psi_+|^2 \, dx = \int_0^1 |c_1|^2 e^{-2x} \, dx = 1 \ ,$$

and

$$\int_0^1 |\psi_-|^2 \, dx = \int_0^1 |c_2|^2 e^{2x} \, dx = 1 \; .$$

Therefore

$$c_1 = \frac{\sqrt{2}e}{\sqrt{e^2-1}} \; ,$$

and

$$c_2 = \frac{\sqrt{2}}{\sqrt{e^2-1}} \; .$$

So normalized solutions are

$$\psi_+(x) = \frac{\sqrt{2}e}{\sqrt{e^2-1}} e^{-x} \; ,$$

and

$$\psi_-(x) = \frac{\sqrt{2}}{\sqrt{e^2-1}} e^{x} \; .$$

Since ψ_+ and ψ_- have equal norms in $L^2(a,b) = L^2(0,1)$, the isometric mappings of F_+ onto F_- are parametrized by γ, where $|\gamma| = 1$ such that

$$\begin{aligned} U_\gamma : \;\; F_+ &\to \;\; F_- \; , \\ \psi_+ &\mapsto \;\; \gamma\psi_- \; . \end{aligned}$$

Let us write the P_{U_γ} as P_γ for simplicity. Theorem 5.17 implies each $\varphi \in D(P_\gamma)$ is of the form

$$\varphi(x) = \varphi_0(x) + \alpha(I - U_\gamma)e^{-x} \; ,$$

where $\varphi_0(x) \in D(P)$, $\alpha \in \mathbb{C}$ and $e^{-x} \in F_+$. Now, we characterize the $D(P_\gamma)$ in terms of the boundary conditions of the functions and show that

$$\begin{aligned} D(P_\gamma) &= \{\varphi = \varphi_0 + \alpha\psi_+ - \alpha\gamma\psi_- : \varphi_0 \in D(P), \alpha \in \mathbb{C}\} \\ &= \{\varphi \in H^1(0,1) : \varphi(1) = \beta\varphi(0) \text{ where } |\beta| = 1\} \; . \end{aligned}$$

In particular $\varphi \in H^1(0,1)$ ($\varphi_0 \in H^1(0,1)$). Since

$$\begin{aligned}\varphi(1) &= \underbrace{\varphi_0(1)}_{0} + \alpha\frac{\sqrt{2}ee^{-1}}{\sqrt{e^2-1}} - \alpha\gamma\frac{\sqrt{2}e}{\sqrt{e^2-1}} \\ &= \alpha\frac{\sqrt{2}ee^{-1}}{\sqrt{e^2-1}} - \alpha\gamma\frac{\sqrt{2}e}{\sqrt{e^2-1}} \ .\end{aligned}$$

Then

$$\varphi(1) = \frac{\sqrt{2}\alpha}{\sqrt{e^2-1}}(1-e\gamma) \ . \tag{5.78}$$

By the same way

$$\varphi(0) = \frac{\sqrt{2}\alpha}{\sqrt{e^2-1}}(e-\gamma) \ . \tag{5.79}$$

The ratio of $\varphi(1)$ with $\varphi(0)$ becomes

$$\frac{\varphi(1)}{\varphi(0)} = \frac{1-e\gamma}{e-\gamma} \ .$$

Notice that

$$\left|\frac{\varphi(1)}{\varphi(0)}\right|^2 = \frac{(1-e\gamma)(1-e\overline{\gamma})}{(e-\gamma)(e-\overline{\gamma})} = \frac{1-e\overline{\gamma}-e\gamma+e^2|\gamma|^2}{e^2-e\overline{\gamma}-e\gamma+|\gamma|^2} = 1 \ .$$

So we get

$$\varphi(1) = \beta\varphi(0) \ ,$$

where $|\beta| = 1$ and $\beta = \frac{1-e\gamma}{e-\gamma}$, that is $\varphi \in H^1(0,1)$ and satisfies the boundary conditions stated above.

Conversely, if $\varphi \in H^1(0,1)$ satisfies Equation 5.78 and setting $\alpha := \varphi(0)\frac{\sqrt{e^2-1}}{\sqrt{2}(e-\gamma)}$ and $\varphi_0 := \varphi(x) - \alpha(1-U_\gamma)\psi_+$, we get

$$\varphi_0(0) = \varphi(0) - \underbrace{\frac{\varphi(0)\sqrt{e^2-1}}{\sqrt{2}(e-\gamma)}}_{\alpha}\left[\frac{\sqrt{2}ee^0}{\sqrt{e^2-1}} - \gamma\frac{\sqrt{2}e^0}{\sqrt{e^2-1}}\right] = 0 \ . \tag{5.80}$$

Similarly

$$\begin{aligned}\varphi_0(1) &= \varphi(1) - \frac{\varphi(0)\sqrt{e^2-1}}{\sqrt{2}(e-\gamma)}\left[\frac{\sqrt{2}ee^{-1}}{\sqrt{e^2-1}} - \gamma\frac{\sqrt{2}e^1}{\sqrt{e^2-1}}\right] \\ &= \varphi(1) - \frac{\varphi(0)}{e-\gamma}(1-\gamma e) \\ &= \beta\varphi(0) - \varphi(0)\frac{1-e\gamma}{e-\gamma} \\ &= \frac{1-e\gamma}{e-\gamma}\varphi(0) - \varphi(0)\frac{1-e\gamma}{e-\gamma} = 0 \ .\end{aligned}$$

Hence

$$D(P_\gamma) = \{\varphi \in H^1(0,1) : \varphi(1) = \beta\varphi(0)\} \tag{5.81}$$

where

$$\beta = \frac{1-e\gamma}{e-\gamma} \ , \tag{5.82}$$

with $|\beta| = 1$ and $|\gamma| = 1$. Also notice that above equation is a bijection between γ and β with the inverse

$$\gamma = \frac{1-e\beta}{e-\beta} \ . \tag{5.83}$$

5.5. Dirac Delta Potential in One-Dimension

In this section, we first give a formal discussion of a well-known quantum mechanical problem, where the potential is given by Dirac delta function (Griffiths and Schroeter, 2018). Then, we go back to the same problem from the self-adjoint extension point of view, which makes the Hamiltonian operator of the system well-defined.

The Schrödinger equation for this system is given by

$$(H\varphi)(x) = -\frac{h^2}{2m}\frac{d^2\varphi(x)}{dx^2} - g\delta(x)\varphi(x) = E\varphi(x) \ ,$$

where $g > 0$ (coupling constant). We now consider the bound state problem for the system, that is,

$$E = -\nu^2 \ ,$$

where $\nu > 0$. Moreover, we will use the units such that $\hbar = 1$, $2m = 1$. In this case, we have

$$-\frac{d^2\varphi(x)}{dx^2} - g\delta(x)\varphi(x) = -\nu^2\varphi(x) \ . \tag{5.84}$$

We imagine that the support of the potential is at the origin so that we can split the region into two sub region, where $x < 0$ and $x > 0$. The idea is based on the following argument:

We shall solve the differential equation (Equation (5.84)) for two regions and then apply the so-called matching condition at $x = 0$.

For $x < 0$: We imagine that $V(x) = 0$ for $x < 0$ (since we are outside of the support). Then, Equation (5.84) becomes

$$-\frac{d^2\varphi_1(x)}{dx^2} = -\nu^2\varphi_1(x) \ .$$

Then the general solution is

$$\varphi_1(x) = Ae^{-\nu x} + Be^{\nu x} \ , \tag{5.85}$$

for $x < 0$. Similarly for $x > 0$

$$\varphi_2(x) = Ce^{-\nu x} + De^{\nu x} \ . \tag{5.86}$$

Since we are interested in the study of bound states, we need to impose the condition $\varphi(x)$ as $|x| \to \infty$ to the general solutions $\varphi_1(x)$ and $\varphi_2(x)$. Then, we must have

$$A = D = 0 \ .$$

Hence the solution for $x < 0$

$$\varphi_1(x) = Be^{\nu x} \ , \tag{5.87}$$

and the solution for $x > 0$

$$\varphi_2(x) = Ce^{-\nu x} \ . \tag{5.88}$$

It remains to impose the matching conditions. The first matching condition is the continuity of the wave functions at $x = 0$, namely

$$\lim_{\epsilon \to 0^-} \varphi_1(\epsilon) = \lim_{\epsilon \to 0^+} \varphi_2(\epsilon) \ . \tag{5.89}$$

The second matching condition is

$$\lim_{\epsilon \to 0} \left(\left. \frac{d\varphi(x)}{dx} \right|_{\epsilon} - \left. \frac{d\varphi(x)}{dx} \right|_{-\epsilon} \right) = -g\varphi(0) \ . \tag{5.90}$$

Let us show this by integrating the Schrödinger equation (Equation (5.84)) from $-\epsilon$ to ϵ, where $\epsilon > 0$.

$$\begin{aligned} -\int_{-\epsilon}^{\epsilon} \varphi''(x)\ dx - g \int_{-\epsilon}^{\epsilon} \delta(x)\varphi(x)\ dx &= -\nu^2 \int_{-\epsilon}^{\epsilon} \varphi(x)\ dx \\ -\varphi'(x) \Big|_{-\epsilon}^{\epsilon} - g\varphi(0) &= -\nu^2 \int_{-\epsilon}^{\epsilon} \varphi(x)\ dx \\ -\left(\left. \frac{d\varphi(x)}{dx} \right|_{\epsilon} - \left. \frac{d\varphi(x)}{dx} \right|_{-\epsilon} \right) - g\varphi(0) &= -\nu^2 \int_{-\epsilon}^{\epsilon} \varphi(x)\ dx \ . \end{aligned}$$

Taking the limits as $\epsilon \to 0$, right hand side is going to zero (the wave function φ is continuous). Therefore we get the condition (5.90).

Let us now apply the matching conditions (5.89) and (5.90) for our solutions (5.87) and (5.88).

From the first matching condition, we get

$$B = C = \varphi(0) \ . \tag{5.91}$$

From the second matching condition, we get

$$-2B\nu = g\varphi(0) \ . \tag{5.92}$$

Substituting Equation (5.91) into Equation (5.92), we get $\nu = \frac{g}{2}$, that is,

$$E = -\nu^2 = -\frac{g^2}{4} \ , \tag{5.93}$$

which is the bound state energy. The bound state wave function is

$$\varphi(x) = \begin{cases} Be^{\frac{g}{2}x}, & x < 0 \\ Be^{-\frac{g}{2}x}, & x > 0 \end{cases} .$$

The constant B can be found from the normalization condition and obtain

$$B = \sqrt{\frac{g}{2}} \ .$$

Hence

$$\varphi(x) = \sqrt{\frac{g}{2}} e^{-\frac{g}{2}|x|} \ . \tag{5.94}$$

One can also study the scattering problem, but we will not discuss the scattering in this thesis.

Now, we will approach the same problem from the Von Neumann's self-adjoint extensions (Thirring, 2013). In order to make sense of adding a delta potential to the free Hamiltonian, we start with the following free Hamiltonian

$$H = -\frac{d^2}{dx^2} \ ,$$

where

$$D(H) = \{\varphi(x) \in L^2(\mathbb{R}) : \varphi' \in AC \text{ and } \varphi'' \in L^2(\mathbb{R}), \text{and } \varphi(0) = 0\} \ . \tag{5.95}$$

The conditions of absolutely continuity of φ and $\varphi(0) = 0$ guarantee that H is symmetric on $D(H)$. Taking the Fourier Transformation of H (see Appendix B), we get

$$(\hat{H}\hat{\varphi})(p) = p^2\hat{\varphi}(p) \ , \tag{5.96}$$

where

$$D(\hat{H}) = \left\{\hat{\varphi} \in L^2\left(\mathbb{R}; \frac{dp}{2\pi}\right) : \int_{-\infty}^{\infty} p^4|\hat{\varphi}(p)|^2 \, \frac{dp}{2\pi} < \infty \text{ and } \int_{-\infty}^{\infty} \hat{\varphi}(p) \, \frac{dp}{2\pi} = 0\right\} .$$

This is an another characterization of the initial domain given above (5.95) in terms of Fourier transformation.

First, let us show that $\hat{H}$ defined on $D(\hat{H})$ is not self-adjoint by using Theorem 4.20 (iii). If the operator $\hat{H}$ was self-adjoint, the following equation would hold for all $\hat{\psi} \in D(\hat{H})$:

$$(\hat{H} \pm iI)\hat{\varphi} = (p^2 \pm iI)\hat{\varphi} = \hat{\psi} \ , \tag{5.97}$$

and the solution would be

$$\hat{\varphi}(p) = \frac{\hat{\psi}(p)}{p^2 \pm i} \ . \tag{5.98}$$

But the solution $\hat{\varphi} \notin D(\hat{H})$ for general $\hat{\psi} \in L^2(\mathbb{R})$. So the Equation (5.97) is not satisfied for all $\hat{\psi} \in L^2(\mathbb{R})$.

In order to show $\hat{H}$ is closed on its domain. Recall the Proposition 3.28 which says that the operator $\hat{H}$ is closed if only if $D(\hat{H})$ is complete with respect to its graph norm, where the graph norm is defined as follows:

$$||\hat{\varphi}||_\Gamma^2 := ||\hat{\varphi}||_{L^2}^2 + ||\hat{H}\hat{\varphi}||_{L^2}^2 \ .$$

Using (5.96), we get

$$\langle\hat{\varphi}, \hat{\varphi}\rangle_\Gamma = \int_{-\infty}^{\infty} |\hat{\varphi}(p)|^2 \, \frac{dp}{2\pi} + \int_{-\infty}^{\infty} p^4|\hat{\varphi}(p)|^2 \, \frac{dp}{2\pi} = \int_{-\infty}^{\infty} \overline{\hat{\varphi}(p)}\hat{\varphi}(p) \, \frac{(1+p^4)dp}{2\pi} \ .$$

We can reformulate the $D(\hat{H})$ using the graph norm as follows:

$$D(\hat{H}) = \left\{ \hat{\varphi}(p) \in L^2 \left(\mathbb{R}; \frac{dp}{2\pi} \right) \, : \, ||\hat{\varphi}||_\Gamma < \infty \text{ and } \langle \hat{\varphi}, \frac{1}{1+p^4} \rangle_\Gamma = 0 \right\} ,$$

since

$$0 = \int_{-\infty}^{\infty} \hat{\varphi}(p) \, \frac{dp}{2\pi} = \int_{-\infty}^{\infty} \overline{\hat{\varphi}(p)} \, \frac{dp}{2\pi} = \int_{-\infty}^{\infty} \overline{\hat{\varphi}(p)} \frac{1}{1+p^4} (1+p^4) \, \frac{dp}{2\pi} = \langle \hat{\varphi}, \frac{1}{1+p^4} \rangle_\Gamma ,$$

where we have used $\int_{-\infty}^{\infty} \left(\frac{1}{1+p^4} \right)^2 \, \frac{dp}{2\pi} < \infty$. Since the graph norm and graph inner product is continuous, $D(\hat{H})$ is complete with respect to the graph norm. This means that $\hat{H}$ is closed on $D(\hat{H})$.

In order to find the self-adjoint extension of this operator, we need to find $d_+(\hat{H})$ and $d_-(\hat{H})$, that is,

$$\begin{aligned} d_+(\hat{H}) &= dim[Ker(\hat{H}^* - i)] = dim(F_+) \\ d_+(\hat{H}) &= dim[Ker(\hat{H}^* + i)] = dim(F_-) \, . \end{aligned}$$

For $dim(F_+)$: Suppose $(\hat{H}^* - i)\hat{\psi} = 0$, then

$$0 = \langle \hat{H}^* - i)\hat{\psi}, \hat{\varphi} \rangle = \langle \hat{\psi}, (\hat{H} + i)\hat{\varphi} \rangle = \int_{-\infty}^{\infty} \overline{\hat{\psi}}(p) \, \hat{\varphi}(p) \, (p^2 + i) \, \frac{dp}{2\pi} ,$$

for all $\hat{\varphi} \in D(\hat{H})$. By definition of $D(\hat{H})$

$$\int_{-\infty}^{\infty} \hat{\varphi}(p) \, \frac{dp}{2\pi} = 0 ,$$

so $\hat{\psi}(p) = \frac{1}{p^2 - i}$. There will be no other solutions (suppose there is another solution, say $\hat{\psi}_2$. Then, by the denseness of $\hat{\varphi}$ with respect to L^2 norm, we get the desired result). In coordinate space, by using inverse Fourier Transform and by choosing the contour as the semi circle in the complex upper half plane for $x > 0$ and the semi circle in the complex lower half plane for $x < 0$, the contour integration from residue theorem gives (poles are at $\pm e^{i\pi/4}$)

$$\psi(x) = c_1 e^{-\frac{|x|}{\sqrt{2}}(1-i)} \ .$$

where we have used the Jordan lemma (Brown et al., 2009). Therefore $dim(F_+) = 1$.

Similarly $\hat{\psi}(p) = \frac{1}{p^2+i}$ for F_- and $\psi(x) = c_2 e^{-\frac{|x|}{\sqrt{2}}(1+i)}$. So $dim(F_-) = 1$. Since $dim(F_-) = dim(F_+) = 1$, there is a 1-parameter family of self-adjoint extension of the Hamiltonian. Then, the isometric mapping U of F_+ onto F_- must be in the following form: $\psi_+ \mapsto \gamma\psi_-$, where $|\gamma| = 1$. From the Theorem 5.17 (Von Neumann's theorem on self-adjoint extensions), each function in the domain of $D(H_\gamma)$ is of the form:

$$\varphi(x) = \varphi_0(x) + \alpha(I - U_\gamma)\psi_+ \ , \tag{5.99}$$

where $\varphi_0 \in D(H)$. In other words, we have

$$\varphi(x) = \varphi_0(x) + \alpha(e^{-|x|(1+i)/\sqrt{2}} - e^{2i\delta}\ e^{-|x|(1-i)/\sqrt{2}}) \ . \tag{5.100}$$

It is easy to check that $\varphi(0) = 1 - e^{2i\delta}$, where $\delta > 0$. We can also find the characterization of the domain in terms of the boundary conditions. It is a simple exercise that we have

$$\lim_{\epsilon \to 0} \left(\frac{d\varphi(x)}{dx}\bigg|_{\epsilon} - \frac{d\varphi(x)}{dx}\bigg|_{-\epsilon} \right) = -\sqrt{2}(1 - \cot\delta)\varphi(0) \ . \tag{5.101}$$

This is exactly the second matching condition with (5.90) as long as $g = \sqrt{2}(1 - \cot\delta)$.

There are several examples for self-adjoint extensions and approaches to define Dirac delta potentials (e.g., via quadratic forms (De Oliveira, 2008), Krein's resolvent formula (Albeverio and Kurasov, 2000), boundary triplet method (De Oliveira, 2008) and (Schmüdgen, 2012)), see (De Oliveira, 2008) for various examples. In this thesis, we shall consider the two dimensional version of this problem. However, we shall define the model using a different approach expressed by the resolvents.

CHAPTER 6

TWO PARTICLES INTERACTING WITH POINT INTERACTIONS IN THE PLANE

The Hydrogen atom is one of the well-known quantum mechanical two-particle problem, and its solution can be found in any standard textbook of quantum mechanics (Shankar, 2012). In this chapter, we are going to consider another two-particle problem, where the particles are interacting with each other through the point like Dirac delta function in the plane. As summarized in the introduction, there are several approaches for this problem. Here we are going to review the method introduced in (Dimock and Rajeev, 2004). The main idea of this method is to show that the Hamiltonian after the so-called coupling constant renormalization defines a self-adjoint operator. Since we shall deal with only one particular resolvent associated with Hamiltonian operator H, we choose the convention $R_z(H) := R(z)$ throughout this chapter.

Before discussing the point interactions in two dimensions, we first quickly recall the two-body problem in standard quantum mechanics (Shankar, 2012).

6.1. The Two Particle Problem in Quantum Mechanics

We consider two particles interacting with each other in $\mathbb{R}^2$ by some potential (the same analysis can be made in $\mathbb{R}^3$ as well). We suppose that the classical energy of the system is given by the form

$$E = \frac{m_1}{2}\left(\frac{d\mathbf{x}_1}{dt}\right)^2 + \frac{m_2}{2}\left(\frac{d\mathbf{x}_2}{dt}\right)^2 + V(\mathbf{x}_2 - \mathbf{x}_1), \tag{6.1}$$

where $\mathbf{x}_j \in \mathbb{R}^2$ are the position vectors of the j-th particle of mass m_j and $j = 1, 2$. Here, V is assumed to be the potential energy between the particles, describing the interaction among them.

Such mechanical systems described by the above form of energy are extremely important in the motion of celestial bodies - planets, moons, comets, double stars, etc. Using the third law of Newton, the equations of motion are given

$$m_1 \frac{d^2\mathbf{x}_1}{dt^2} = -\mathbf{F} \ , \tag{6.2}$$

$$m_2 \frac{d^2\mathbf{x}_2}{dt^2} = \mathbf{F} \ , \tag{6.3}$$

where $\mathbf{F}$ is the force acting on the one particle due to the other one. As we have emphasized above, we need the specification of four quantities; the two components of each of two position vectors $\mathbf{x}_1$ and $\mathbf{x}_2$. Alternatively, we may define the following point transformation $\mathbb{R}^4 \to \mathbb{R}^4$: the center of mass vector

$$\mathbf{R} = \frac{m_1\mathbf{x}_1 + m_2\mathbf{x}_2}{M} \ , \tag{6.4}$$

called the center of mass, and

$$\mathbf{r} = \mathbf{x}_2 - \mathbf{x}_1 \ , \tag{6.5}$$

called the relative coordinate. The length of the relative coordinate is denoted by r. Using these, we can find

$$\mathbf{x}_1 = \mathbf{R} - \frac{m_2}{M}\mathbf{r} \ , \tag{6.6}$$

and

$$\mathbf{x}_2 = \mathbf{R} + \frac{m_1}{M}\mathbf{r} \ . \tag{6.7}$$

Since the center of mass of the system is not accelerating (adding Equation (6.2) and Equation (6.3), $\frac{d^2R}{dt^2} = 0$), we may choose our inertial frame of reference to be the center of mass frame. In this frame the origin for the coordinate system become the center of mass of the particles, i.e.,

$$\mathbf{R} \equiv \mathbf{0} \ . \tag{6.8}$$

Then,

$$m_1\mathbf{x}_1 + m_2\mathbf{x}_2 = \mathbf{0} \ . \tag{6.9}$$

So, Equations (6.6) and (6.7) are reduced to

$$\mathbf{x}_1 = \frac{m_2}{m_1 + m_2}\mathbf{r} , \quad (6.10)$$

$$\mathbf{x}_2 = -\frac{m_1}{m_1 + m_2}\mathbf{r} . \quad (6.11)$$

Substituting these into the Equation (6.1), we obtain

$$E = \frac{1}{2}\mu|\mathbf{r}|^2 + V(\mathbf{r}) , \quad (6.12)$$

where

$$\mu := \frac{m_1 m_2}{m_1 + m_2} \quad (6.13)$$

is called the reduced mass.

Hence, we formally reduced the problem of the motion of two particles to an equivalent one-particle problem, where we have a fictitious particle with mass μ moving in a central field $V(\mathbf{r})$. Then, the reduced problem is easier to solve, see e.g., Kepler problem in classical mechanics (Marion, 2013).

From the canonical quantization procedure (principle 2 of quantum mechanics that is given in Chapter 2) we replace $\mathbf{p}_1 = (p_{1,1}, p_{1,2})$, $\mathbf{p}_2 = (p_{2,1}, p_{2,2})$, $\mathbf{x}_1 = (x_{1,1}, x_{1,2})$ and $\mathbf{x}_2 = (x_{2,1}, x_{2,2})$ by self-adjoint operators P_1 , P_2 , X_1 and X_2, defined by

$$(P_j\psi)(\mathbf{x}_1, \mathbf{x}_2) := -i\hbar\left(\frac{\partial}{\partial x_{j,1}}, \frac{\partial}{\partial x_{j,2}}\right)\psi = -i\hbar\nabla_j\psi , \quad (6.14)$$

and

$$(X_j\psi)(\mathbf{x}_1, \mathbf{x}_2) = \mathbf{x}_j\psi(\mathbf{x}_1, \mathbf{x}_2) \quad (6.15)$$

in $L^2(\mathbb{R}^2 \times \mathbb{R}^2) = L^2(\mathbb{R}^4)$. Here $\psi(\mathbf{x}_1, \mathbf{x}_2) = \psi(x_{1,1}, x_{1,2}, x_{2,1}, x_{2,2})$ and the first index represents the particle label and the second index represents the components.

With this association, the energy observable, namely the quantum Hamiltonian, is given by

$$H = -\frac{\Delta_1}{2} - \frac{\Delta_2}{2} + V(\mathbf{x}_2 - \mathbf{x_1}) , \quad (6.16)$$

where Δ_j is the Laplacian acting on functions with j the particle variables $\mathbf{x}_j$, i.e.,

$$\Delta_j = \Delta_{\mathbf{x}_j} := -\left(\frac{\partial^2}{\partial x_{j,1}^2} + \frac{\partial^2}{\partial x_{j,2}^2}\right) , \tag{6.17}$$

and we have used the units such that $m_1 = m_2 = \hbar = 1$ for simplicity.

If there is no interaction between particles, Hamiltonian is represented by H_0 (free Hamiltonian)

$$H_0 = -\frac{\Delta_1}{2} - \frac{\Delta_2}{2} . \tag{6.18}$$

The reduction of the two-particle problem to one-particle in quantum mechanics can be similarly made. We can find Δ_1 and Δ_2 in the relative and center of mass coordinates.

Using the chain rule, we have

$$\frac{\partial}{\partial x_{1,1}} = -\frac{\partial}{\partial r_1} + \frac{1}{2}\frac{\partial}{\partial R_1} ,$$

and

$$\frac{\partial}{\partial x_{1,2}} = -\frac{\partial}{\partial r_2} + \frac{1}{2}\frac{\partial}{\partial R_2} .$$

Then we get

$$\frac{\partial^2}{\partial x_{1,1}^2} = \frac{\partial^2}{\partial r_1^2} - \frac{1}{2}\frac{\partial^2}{\partial r_1 R_1} - \frac{1}{2}\frac{\partial^2}{\partial R_1 r_1} + \frac{1}{4}\frac{\partial^2}{\partial R_1^2} , \tag{6.19}$$

$$\frac{\partial^2}{\partial x_{1,2}^2} = \frac{\partial^2}{\partial r_2^2} - \frac{1}{2}\frac{\partial^2}{\partial r_2 R_2} - \frac{1}{2}\frac{\partial^2}{\partial R_2 r_2} + \frac{1}{4}\frac{\partial^2}{\partial R_2^2} . \tag{6.20}$$

Similarly, one can find

$$\frac{\partial^2}{\partial x_{2,1}^2} = \frac{\partial^2}{\partial r_1^2} + \frac{1}{2}\frac{\partial^2}{\partial r_1 R_1} + \frac{1}{2}\frac{\partial^2}{\partial R_1 r_1} + \frac{1}{4}\frac{\partial^2}{\partial R_1^2} , \tag{6.21}$$

$$\frac{\partial^2}{\partial x_{2,2}^2} = \frac{\partial^2}{\partial r_2^2} + \frac{1}{2}\frac{\partial^2}{\partial r_2 R_2} + \frac{1}{2}\frac{\partial^2}{\partial R_2 r_2} + \frac{1}{4}\frac{\partial^2}{\partial R_2^2} . \tag{6.22}$$

Therefore, the sum of equations (6.19), (6.20), (6.21) and (6.22) becomes

$$\Delta_1 + \Delta_2 = 2\left(\frac{\partial^2}{\partial r_1^2} + \frac{\partial^2}{\partial r_2^2}\right) + \frac{1}{2}\left(\frac{\partial^2}{\partial R_1^2} + \frac{\partial^2}{\partial R_2^2}\right) . \tag{6.23}$$

By setting

$$\Delta_{\mathbf{r}} := \frac{\partial^2}{\partial r_1^2} + \frac{\partial^2}{\partial r_2^2} , \tag{6.24}$$

$$\Delta_{\mathbf{R}} := \frac{\partial^2}{\partial R_1^2} + \frac{\partial^2}{\partial R_2^2} , \tag{6.25}$$

we get the transformed Hamiltonian

$$H' := -\Delta_{\mathbf{r}} - \frac{1}{4}\Delta_{\mathbf{R}} + V(\mathbf{r}) . \tag{6.26}$$

Now our aim is to solve the following Shrödinger equation

$$H'\psi(\mathbf{r},\mathbf{R}) = \left[- \Delta_{\mathbf{r}} - \frac{1}{4}\Delta_{\mathbf{R}} + V(\mathbf{r})\right]\psi(\mathbf{r},\mathbf{R}) = E\psi(\mathbf{r},\mathbf{R}) . \tag{6.27}$$

Let us now use the separation of variables, that is, $\psi(\mathbf{r},\mathbf{R}) = \psi_1(\mathbf{r})\psi_2(\mathbf{R})$. For simplicity we will call this product as $\psi_1\psi_2$. Hence, we get

$$-\psi_2\Delta_{\mathbf{r}}\psi_1 - \frac{\psi_1}{4}\Delta_{\mathbf{R}}\psi_2 + V(\mathbf{r})\psi_1\psi_2 = E\psi_1\psi_2 . \tag{6.28}$$

Dividing both sides by $\psi_1\psi_2$, we have

$$-\frac{1}{\psi_1(\mathbf{r})}\Delta_{\mathbf{r}}\psi_1(\mathbf{r}) + V(\mathbf{r}) - \frac{1}{4\psi_2(\mathbf{R})}\Delta_{\mathbf{R}}\psi_2(\mathbf{R}) = E . \tag{6.29}$$

The first two terms on the left hand side is a function of $\mathbf{r}$ whereas the last term is a function of $\mathbf{R}$. So this equation can only make sense only when each term is equal to some constant, namely E_1 and E_2 respectively. Hence we get two uncoupled partial differential equations:

$$-\frac{1}{\psi_1(\mathbf{r})}\Delta_{\mathbf{r}}\psi_1(\mathbf{r}) + V(\mathbf{r}) = E_1 \ , \tag{6.30}$$

and

$$-\frac{1}{4\psi_2(\mathbf{R})}\Delta_{\mathbf{R}}\psi_2(\mathbf{R}) = E_2 \ , \tag{6.31}$$

where $E_1 + E_2 = E$. The equations (6.30) and (6.31) can be rewritten in the following form:

$$H_{rel}\psi_1 = E_1\psi_1 \ , \tag{6.32}$$

and

$$H_{CM}\psi_2 = E_2\psi_2 \ , \tag{6.33}$$

where

$$H_{rel} := -\Delta_{\mathbf{r}} + V(\mathbf{r}) \ , \tag{6.34}$$

$$H_{CM} := -\frac{1}{4}\Delta_{\mathbf{R}} \ . \tag{6.35}$$

The non-trivial part of the problem is now encoded only in the Hamiltonian H_{rel}, since this is the only equation which includes the interaction term $V(\mathbf{r})$. For this reason, we will relabel $H_{rel} = H$ and $\psi_1 = \psi$ for simplicity. Hence, we shall write Hamiltonian in relative coordinates as:

$$H = -\Delta_{\mathbf{r}} + V(\mathbf{r}) \ . \tag{6.36}$$

Sometimes, we shall denote $-\Delta_{\mathbf{r}}$ as the free Hamiltonian, i.e.,

$$-\Delta_{\mathbf{r}} := H_0 \ . \tag{6.37}$$

We shall assume that this operator is defined on the following domain

$$D(H_0) = D(-\Delta) = \{\psi \in L^2(\mathbb{R}^2) : |\mathbf{k}|^2\hat{\psi}(\mathbf{k}) \in L^2(\mathbb{R}^2)\} \ , \tag{6.38}$$

where

$$-\Delta\psi = \mathcal{F}^{-1}(|\mathbf{k}|^2\hat{\psi}(\mathbf{k})) \;, \tag{6.39}$$

where $\hat{\psi}$ is the Fourier transform of ψ (See Appendix B) and $\mathcal{F}^{-1}$ is the inverse Fourier transformation. Equivalently, $D(-\Delta)$ can also be described as the set of all $\psi \in L^2(\mathbb{R}^2)$ such that $\Delta\psi \in L^2(\mathbb{R}^2)$ in the distributional sense, namely the Sobolev space $H^2(\mathbb{R}^2)$ (see page 188 in (Hall, 2013)). By following the same approach given in Example 5.18 for the momentum operator, it is easy to show that the free Hamiltonian on the above domain is self-adjoint.

If we have more than two particles or identical particles, it is useful to consider the above formalism in tensor product spaces (the tensor product of two Hilbert spaces is defined as follows: Suppose $\varphi_1 \in \mathcal{H}_1$ and $\varphi_2 \in \mathcal{H}_2$. For each φ_1 and φ_2, we define a map $\varphi_1 \otimes \varphi_2 : \mathcal{H}_1 \times \mathcal{H}_2 \to \mathbb{C}$ such that $(\varphi_1 \otimes \varphi_2)(\psi_1, \psi_2) := \langle \psi_1, \varphi_1 \rangle \langle \psi_2, \varphi_2 \rangle$ is conjugate bilinear form. The set of all such bilinear forms is a vector space and one can define the following inner product on such a space: $\langle \varphi \otimes \psi, \eta \otimes \mu \rangle := \langle \varphi, \eta \rangle \langle \psi, \mu \rangle$. $\mathcal{H}_1 \otimes \mathcal{H}_2$ is the completion of this space. Moreover, one can define the action of a bounded operator on this space by $(T \otimes S)(\varphi_1 \otimes \varphi_2) := T\varphi_1 \otimes S\varphi_2$, where T act on $\mathcal{H}_1$ and S act on $\mathcal{H}_2$. This construction can be extended to unbounded self-adjoint operators as well (see, e.g., (Reed and Simon, 1972)).

The Hamiltonian H' in Equation (6.26) defined on a tensor product space $L^2(\mathbb{R}^2)$ $\otimes L^2(\mathbb{R}^2)$ under the natural correspondence (isomorphism)

$$L^2(\mathbb{R}^2) \otimes L^2(\mathbb{R}^2) \quad \longleftrightarrow \quad L^2(\mathbb{R}^4) \;, \tag{6.40}$$

where the identification is given by a unitary operator which send the vector $\psi \otimes \phi \in L^2(\mathbb{R}^2) \otimes L^2(\mathbb{R}^2)$ to the function $\psi \otimes \phi \in L^2(\mathbb{R}^4)$ defined as (see (Dimock, 2011))

$$(\psi \otimes \phi)(\mathbf{r}, \mathbf{R}) = \psi(\mathbf{r})\phi(\mathbf{R}) \;. \tag{6.41}$$

With this identification, we can identify the Hamiltonian

$$H' = (H \otimes I) + (I \otimes H_{CM}) \;, \tag{6.42}$$

with $-\Delta_{\mathbf{r}} - \frac{1}{4}\Delta_{\mathbf{R}} + V(\mathbf{r})$ on $L^2(\mathbb{R}^4)$ as we have introduced before.

6.2. Kato-Rellich Theorem

If we go back to the problem described by the Hamiltonian (6.36), it is not obvious that $H = -\Delta + V$ defined on $D(-\Delta) \cap D(V)$ is again a self-adjoint operator for any given generic potential V. Therefore, we must impose some restrictions on V to make H self-adjoint, namely V must be a "small perturbation" to our initial free self-adjoint Hamiltonian $-\Delta$ defined on a proper domain. The proper rigorous formulation of this question is given by the so-called Kato-Rellich theorem. To state the theorem, we must first need to define what we mean by a "small perturbation" to some self-adjoint operator. One technical definition of small perturbations commonly used in physics literature is called the relative boundedness (a weaker notion than the boundedness):

Definition 6.1 *Let T and S be linear operators on $\mathcal{H}$. We say that S is relatively T-bounded if $D(T) \subseteq D(S)$ and there exists nonnegative real numbers a and b such that*

$$||S\psi|| \leq a||T\psi|| + b||\psi|| \; , \tag{6.43}$$

for all $\psi \in D(T)$. The infimum of all the non-negative numbers a for which there exists a non-negative number b such that the above inequality (6.43) holds is called T-bound of S, denoted by $\alpha_T(S)$.

Theorem 6.2 (Kato-Rellich Theorem) *Let T be a self-adjoint operator on $\mathcal{H}$. Suppose that S is a relatively T-bounded symmetric operator on $\mathcal{H}$ with T-bound $\alpha_T(S) < 1$. Then,*

$$T + S$$

on $D(T + S) = D(T)$ is self-adjoint.

Proof: By the assumption of relative boundedness with bound less than 1, we have positive constants a, b with $a < 1$ such that the above inequality (6.43) holds. Since T is self-adjoint, it must be symmetric. As we have seen that every symmetric operator satisfies the Equation (3.42). Therefore, using this equation for $z = -i\lambda$ with $\lambda \in \mathbb{R}$, we have

$$||(T - i\lambda I)\varphi||^2 = ||T\varphi||^2 + |\lambda|^2||\varphi||^2 \ , \tag{6.44}$$

for all $\varphi \in D(T)$. Due to the positivity of each terms on the right hand side, we get the following two inequalities

$$\begin{aligned} ||(T - i\lambda I)\varphi|| &\geq ||T\varphi|| \ , & (6.45) \\ ||(T - i\lambda I)\varphi|| &\geq |\lambda|||\varphi|| \ . & (6.46) \end{aligned}$$

Using these inequalities and relative T-boundedness of S, we have

$$\begin{aligned} ||S\varphi|| &\leq a||T\varphi|| + b||\varphi|| & (6.47) \\ &\leq \underbrace{a||(T - i\lambda I)\varphi|| + b\frac{||(T - i\lambda I)\varphi||}{|\lambda|}}_{=\left(a+\frac{b}{|\lambda|}\right)||(T-i\lambda I)\varphi||} \ . & (6.48) \end{aligned}$$

Since T is self-adjoint operator, then there exists $\varphi \in D(T)$ such that

$$\varphi = (T - i\lambda I)^{-1}\psi \ , \tag{6.49}$$

for any $\psi \in \mathcal{H}$ thanks to the self-adjointness criteria $Ran(T - i\lambda I) = \mathcal{H}$ (Theorem 4.20 and Theorem 4.22). Plugging this into the Equation (6.48), we get

$$||S(T - i\lambda I)^{-1}\psi|| \leq (a + b|\lambda|^{-1})||\psi|| \ , \tag{6.50}$$

for any $\psi \in \mathcal{H}$. Since $a < 1$, $(a + b|\lambda|^{-1}) < 1$ for sufficiently large $|\lambda|$ (since λ was arbitrary). This argument works for the particular case, where the operator T is bounded operator. This corresponds to the case where $a = 0$. This allows us to define the following bounded operator whose norm less than 1:

$$A := S(T - i\lambda I)^{-1} \ , \tag{6.51}$$

where its domain is the full Hilbert space $D(A) = \mathcal{H}$ thanks to the BLT Theorem (Theorem 3.22). Then we can construct the following convergent series formed by bounded operator A

$$\sum_{m=0}^{\infty}(-A)^m \ . \tag{6.52}$$

By Proposition 3.47, the result of this series converges to

$$\sum_{m=0}^{\infty}(-A)^m = (I + A)^{-1} \ . \tag{6.53}$$

This means that $(I + A)$ has a bounded inverse defined on $\mathcal{H}$ so $Ran(I + A) = \mathcal{H}$.

On the other hand, since $Ran(T - i\lambda I) = \mathcal{H}$ we get

$$\underbrace{(I + A)(T - i\lambda I)\varphi}_{\in Ran(I+A)=\mathcal{H}} = (I + S(T - i\lambda I)^{-1})(T - i\lambda I)\varphi \tag{6.54}$$

$$= \underbrace{(T - i\lambda I + S)\varphi}_{\in Ran(T+S-i\lambda I)} \ , \tag{6.55}$$

for any $\varphi \in D(T)$. Then $Ran(T + S - i\lambda I) = \mathcal{H}$ for sufficiently large $|\lambda|$. Therefore by the self-adjointness criteria (Theorem 4.20) and by Theorem 4.22, $T + S$ is self-adjoint (see for instance (Reed and Simon, 1975)). □

Example 6.3 *Let H_0 be the free self-adjoint Hamiltonian defined on $D(H_0)$, described by (6.38). Then, $H = H_0 + V$ on $L^2(\mathbb{R}^n)$ is self-adjoint on $D(H_0)$ in the following cases:*

(i) $V \in L^\infty(\mathbb{R}^n)$ *(measurable functions bounded up to a set of measure zero)* ,

(ii) $V \in L^2(\mathbb{R}^n)$,

(iii) $V = V_1 + V_2$ *for* $V_1 \in L^2(\mathbb{R}^n)$ *and* $V_2 \in L^\infty(\mathbb{R}^n)$*, were* $n = 1, 2, 3$.

The proof of all these cases are consequences of Kato-Rellich theorem, as we are now going to show it. Suppose that $V \in L^\infty$*, then*

$$||V\psi|| = \left(\int_{\mathbb{R}^n} |V(\mathbf{x})\psi(\mathbf{x})|^2 \, d\mathbf{x} \right)^{1/2} \leq \sup_{\mathbf{x}\in\mathbb{R}^n} |V(\mathbf{x})| \left(\int_{\mathbb{R}^n} |\psi(\mathbf{x})|^2 \, d\mathbf{x} \right)^{1/2} = ||V||_\infty ||\psi|| \, .$$

This inequality implies that the operator V *is bounded. Since the boundedness implies the relative boundedness, or the hypothesis of Kato-Rellich's theorem are satisfied with* $a = 0$*,* $b = ||V||_\infty$*, we have shown the first part (i) of the result.*

We now assume that $V \in L^2(\mathbb{R}^n)$*. If* $\psi \in D(H_0)$*, then we must have* $|\mathbf{p}|^2\hat{\psi}(\mathbf{p}) \in L^2(\mathbb{R}^n)$ *(see (6.38)). By writing* $\hat{\psi}(\mathbf{p})$ *as*

$$\hat{\psi}(\mathbf{p}) = (\alpha^2 + |\mathbf{p}|^2)^{-1}(\alpha^2 + |\mathbf{p}|^2)\hat{\psi}(\mathbf{p}) \, , \tag{6.56}$$

for any $\alpha > 0$*, it is easy to see that* $\hat{\psi}(\mathbf{p})$ *can be written as the product of two* $L^2(\mathbb{R}^n)$ *functions, namely* $(\alpha^2 + |\mathbf{p}|^2)^{-1}$ *and* $(\alpha^2 + |\mathbf{p}|^2)\hat{\psi}(\mathbf{p})$*. This means that it must be inside* $L^1(\mathbb{R}^n)$ *as well as* $L^2(\mathbb{R}^n) : L^1(\mathbb{R}^n) \cap L^2(\mathbb{R}^n)$*, which can be easily seen from the Cauchy-Schwarz inequality (3.3):*

$$\left| \int_{\mathbb{R}^n} \overline{f(\mathbf{p})} g(\mathbf{p}) \, \frac{d\mathbf{p}}{(2\pi)^n} \right| \leq \left(\int_{\mathbb{R}^n} |f(\mathbf{p})|^2 \, \frac{d\mathbf{p}}{(2\pi)^n} \right)^{1/2} \left(\int_{\mathbb{R}^n} |g(\mathbf{p})|^2 \, \frac{d\mathbf{p}}{(2\pi)^n} \right)^{1/2} , \tag{6.57}$$

where $f(\mathbf{p}) = (\alpha^2 + |\mathbf{p}|^2)^{-1}$ *and* $g(\mathbf{p}) = (\alpha^2 + |\mathbf{p}|^2)\hat{\psi}(\mathbf{p})$*. Hence the Fourier inversion formula is valid and*

$$\psi(\mathbf{x}) = \int_{\mathbb{R}^n} e^{i\mathbf{p}\cdot\mathbf{x}} \hat{\psi}(\mathbf{p}) \, \frac{d\mathbf{p}}{(2\pi)^n} \tag{6.58}$$

holds pointwise (See Appendix B, Fourier Transform on L^2 (Hall, 2013)). Then, we have

$$|\psi(\mathbf{x})| = \left| \int_{\mathbb{R}^n} e^{i\mathbf{p}\cdot\mathbf{x}} \hat{\psi}(\mathbf{p}) \frac{d\mathbf{p}}{(2\pi)^n} \right| \leq \int_{\mathbb{R}^n} \left| \hat{\psi}(\mathbf{p}) \right| \frac{d\mathbf{p}}{(2\pi)^n} \tag{6.59}$$

$$\leq \left(\int_{\mathbb{R}^n} (\alpha^2 + |\mathbf{p}|^2)^{-2} \frac{d\mathbf{p}}{(2\pi)^n} \right)^{1/2} \left(\int_{\mathbb{R}^n} (\alpha^2 + |\mathbf{p}|^2)^2 |\hat{\psi}(\mathbf{p})|^2 \frac{d\mathbf{p}}{(2\pi)^n} \right)^{1/2} . \tag{6.60}$$

Let us explicitly show that the integrals $\int_{\mathbb{R}^n} (\alpha^2 + |\mathbf{p}|^2)^{-2} \frac{d\mathbf{p}}{(2\pi)^n}$ *are convergent.*

For $n = 1$, it is easy to see that

$$\int_{\mathbb{R}} (\alpha^2 + |p|^2)^{-2} \frac{dp}{2\pi} = \frac{1}{4\alpha^3} . \tag{6.61}$$

For $n = 2$, we go to the polar coordinates and evaluate the integral as

$$\int_{\mathbb{R}^2} (\alpha^2 + |\mathbf{p}|^2)^{-2} \frac{d\mathbf{p}}{(2\pi)^2} = \frac{1}{(2\pi)} \int_0^\infty (\alpha^2 + |p|^2)^{-2} p \, dp = \frac{1}{4\pi\alpha^2} . \tag{6.62}$$

For $n = 3$, we go to the spherical coordinates and evaluate the integral as

$$\int_{\mathbb{R}^3} (\alpha^2 + |\mathbf{p}|^2)^{-2} \frac{d\mathbf{p}}{(2\pi)^3} = \frac{4\pi}{(2\pi)^3} \int_0^\infty (\alpha^2 + |p|^2)^{-2} p^2 \, dp = \frac{1}{8\pi\alpha} . \tag{6.63}$$

Hence, we get

$$|\psi(\mathbf{x})| \leq c_n \alpha^{(n-4)/2} ||(H_0 + \alpha^2)\psi|| \tag{6.64}$$

$$\leq c_n \alpha^{(n-4)/2} ||H_0 \psi|| + c_n \alpha^{n/2} ||\psi|| , \tag{6.65}$$

where c_n's are the square roots of the constants in front of the factors α in the above integrals. This implies that the function $\psi(\mathbf{x})$ is bounded, so it is inside the domain of V (since bounded functions are in $L^2(\mathbb{R}^n)$). According to above inequality, if $\psi \in D(H_0)$, *then $\psi \in D(V)$, i.e., $D(H_0) \subseteq D(V)$. Furthermore for $\psi \in D(H_0)$ we have*

$$||V\psi|| \leq ||V|| ||\psi||_\infty \leq ||V||(c_n \alpha^{(n-4)/2}||H_0\psi|| + c_n \alpha^{n/2}||\psi||) \; . \tag{6.66}$$

Therefore, for sufficiently small α, Kato-Rellich's inequality holds so we conclude that H is self-adjoint on $D(H_0)$.

For the last part of the example, we will treat V_2 as a bounded perturbation of $H_0 + V_1$. Here $D(H_0 + V_1) = D(H_0) \cap \underbrace{D(V_1)}_{=L^2} = D(H_0)$.

As a concrete example, Yukawa potential $V(\mathbf{x}) = \frac{c}{|\mathbf{x}|} e^{-\mu|\mathbf{x}|}$, which is a model of nuclear forces transmitted by a particle of mass $\mu > 0$, and the Coulomb potential $V(\mathbf{x}) = -\frac{e^2}{|\mathbf{x}|}$, which is a simple model of Hydrogen atom are two such class of potentials (see (Dimock, 2011) for the details).

6.3. Two Particles Interacting through the Dirac Delta Potential

In this section, we shall discuss the main topic of this thesis. We consider two particles interacting with each other through the Dirac delta "function" potential in the plane (it can be extended to the three dimensional space as well). According to the result of the previous section, the formal Hamiltonian operator is given by

$$(H\psi)(\mathbf{x}) = -\Delta\psi(\mathbf{x}) - g\delta(\mathbf{x})\psi(\mathbf{x}) \; , \tag{6.67}$$

where $g > 0$ is the strength of the potential, also called coupling constant. The positivity of g implies that the interaction is considered to be attractive. Actually, the subject of such class of singular problems are not new and have been summarized in the Introduction. Here we are going to study this system in detail using the approach introduced in the paper (Dimock and Rajeev, 2004).

The formal Fourier transform of the Hamiltonian given in Equation (6.67) becomes

$$\hat{H}\hat{\psi}(\mathbf{p}) = \mathbf{p}^2\hat{\psi}(\mathbf{p}) - g\int_{\mathbb{R}^2}\hat{\psi}(\mathbf{p})\ \frac{d\mathbf{p}}{(2\pi)^2}\ . \tag{6.68}$$

However, this cannot be a linear operator on $L^2(\mathbb{R}^2)$ (on $L^2(\mathbb{R})$, and on $L^2(\mathbb{R}^3)$ as well) due to the second term:

$$\int_{\mathbb{R}^2}\hat{\psi}(\mathbf{p})\ \frac{d\mathbf{p}}{(2\pi)^2} \notin L^2(\mathbb{R}^2)\ . \tag{6.69}$$

Since we expect that every Hamiltonian associated with some physical system must be a self-adjoint operator on L^2, the above formal Hamiltonian associated with idealized point-like interactions, where the de Broglie wavelength of the particles is much larger than the range of the particles, does not make sense.

One possible way to solve this problem is to approximate the above Hamiltonian in some sense. For this purpose, the above formal Hamiltonian is first regularized as

$$(\hat{H}_\Lambda\hat{\psi})(\mathbf{p}) = \mathbf{p}^2\hat{\psi}(\mathbf{p}) - g_\Lambda\chi_\Lambda(\mathbf{p})\int_{\mathbb{R}^2}\chi_\Lambda(\mathbf{q})\hat{\psi}(\mathbf{q})\ \frac{d\mathbf{q}}{(2\pi)^2}\ , \tag{6.70}$$

via the characteristic function $\chi_\Lambda(\mathbf{p})$ of the disc (ball in three dimensions) of radius Λ, i.e.,

$$\chi_\Lambda(\mathbf{p}) = \begin{cases} 1, & |\mathbf{p}| \leq \Lambda \\ 0, & |\mathbf{p}| > \Lambda \end{cases} \tag{6.71}$$

and g_Λ is assumed to be bounded. This step is called cutoff-regularization in the physics literature. We have defined the above approximate Hamiltonian in the above form such that it is symmetric. For simplicity we consider the second term on the right hand side of the Equation (6.70) as the projection operator onto the characteristic function χ_Λ, i.e.,

$$\mathbb{P}_{\chi_\Lambda}\hat{\psi} = \chi_\Lambda\langle\chi_\Lambda, \hat{\psi}\rangle\ , \tag{6.72}$$

where

$$\langle \hat{\psi}, \hat{\varphi} \rangle = \int_{\mathbb{R}^2} \overline{\hat{\psi}(\mathbf{q})} \hat{\varphi}(\mathbf{q}) \, \frac{d\mathbf{q}}{(2\pi)^2} \; . \tag{6.73}$$

Hence

$$\hat{H}_\Lambda = \hat{H}_0 - g_\Lambda \mathbb{P}_{\chi_\Lambda} \; . \tag{6.74}$$

The second term can be interpreted as the rank one (bounded operator with one-dimensional range) perturbation of the free Hamiltonian. Since g_Λ and $\mathbb{P}_{\chi_\Lambda}$ is bounded (see Example 3.16), $\hat{H}_\Lambda$ is a self-adjoint operator on $D(\hat{H}_0)$ thanks to the Kato-Rellich theorem (Theorem 6.2).

Once we regularize the Hamiltonian, the second step is to find the resolvent associated with this regularized Hamiltonian $\hat{H}_\Lambda$:

$$\hat{R}_\Lambda(z) := (\hat{H}_\Lambda - zI)^{-1} \; . \tag{6.75}$$

Let $\hat{R}_0(z) := (\hat{H}_0 - zI)^{-1}$. Here we assume that z must be in the resolvent set of the above operators. For the free part, we know that the resolvent set for H_0 (positive self-adjoint operator) is $\mathbb{C} \setminus [0, \infty)$. From now on, let us remove all the hat symbols for simplicity of the notation. In order to find $R_\Lambda(z)$, we need to solve the following inhomogenous equation (Albeverio and Kurasov, 2000):

$$(H_\Lambda - zI) f = h \; . \tag{6.76}$$

For $\mathrm{Im}(z) \neq 0$, h must be in $L^2(\mathbb{R}^2)$ since $Ran(H_\Lambda - zI) = \mathcal{H} = L^2(\mathbb{R}^2)$ thanks to the self-adjointness of H_Λ (Theorem 4.20 and 4.22). We are going to find f in terms of an operator acting on h, then we match the operator to $(H_\Lambda - zI)^{-1}$. Suppose $\mathrm{Im}(z) > 0$. Since z is in the resolvent set of free Hamiltonian and H_Λ, we can apply $(H_0 - zI)^{-1}$ to the Equation (6.76) from the left, so that we have

$$(H_0 - zI)^{-1} h = (H_0 - zI)^{-1} \left[(H_0 - zI) f - g_\Lambda \chi_\Lambda \langle \chi_\Lambda, f \rangle \right] \; , \tag{6.77}$$

or

$$f = (H_0 - zI)^{-1} h + g_\Lambda \langle \chi_\Lambda, f \rangle (H_0 - zI)^{-1} \chi_\Lambda \; . \tag{6.78}$$

Although we find an expression for f, the right hand side of the Equation (6.78) includes $\langle \chi_\Lambda, f \rangle$, which is unknown. We can find this from the consistency condition by simply taking the inner product of the obtained expression with χ_Λ:

$$\begin{aligned} \langle \chi_\Lambda, f \rangle &= \big\langle \chi_\Lambda, (H_0 - zI)^{-1} h + g_\Lambda \langle \chi_\Lambda, f \rangle (H_0 - zI)^{-1} \chi_\Lambda \big\rangle \\ &= \langle \chi_\Lambda, (H_0 - zI)^{-1} h \rangle + g_\Lambda \langle \chi_\Lambda, f \rangle \langle \chi_\Lambda, (H_0 - zI)^{-1} \chi_\Lambda \rangle \; , \end{aligned}$$

so that

$$\langle \chi_\Lambda, f \rangle = \frac{\langle \chi_\Lambda, (H_0 - zI)^{-1} h \rangle}{1 - g_\Lambda \langle \chi_\Lambda, (H_0 - zI)^{-1} \chi_\Lambda \rangle} \; . \tag{6.79}$$

By plugging the Equation (6.79) into the Equation (6.78), we have

$$f = (H_0 - zI)^{-1} h + g_\Lambda \left(\frac{\langle \chi_\Lambda, (H_0 - zI)^{-1} h \rangle}{1 - g_\Lambda \langle \chi_\Lambda, (H_0 - zI)^{-1} \chi_\Lambda \rangle} \right) (H_0 - zI)^{-1} \chi_\Lambda \; .$$

Therefore, we can read off the resolvent of the regularized Hamiltonian H_Λ

$$R_\Lambda(z) = R_0(z) + \frac{\langle \chi_\Lambda, R_0(z) . \rangle}{g_\Lambda^{-1} - \langle \chi_\Lambda, R_0(z) \chi_\Lambda \rangle} R_0(z) \chi_\Lambda \; . \tag{6.80}$$

Here we have a natural condition

$$\frac{1}{g_\Lambda} \neq \langle \chi_\Lambda, R_0(z) \chi_\Lambda \rangle \; . \tag{6.81}$$

Later we will show what happens when (6.81) does not hold. Since $R_0(z) = (H_0 - z)^{-1}$ is bounded operator on its resolvent set and H_0 is self-adjoint, we have

$$\big((H_0 - zI)^{-1} \big)^* = \big((H_0 - zI)^* \big)^{-1} = (H_0^* - z^* I)^{-1} = (H_0 - \bar{z})^{-1} \; , \tag{6.82}$$

or

$$R_0^*(z) = R_0(\bar{z}) \ . \tag{6.83}$$

Here we have used the Theorem 3.59. Therefore we find

$$R_\Lambda(z) = R_0(z) + \frac{1}{g_\Lambda^{-1} - \langle \chi_\Lambda, R_0(z)\chi_\Lambda \rangle} \langle R_0(\bar{z})\chi_\Lambda, . \rangle R_0(z)\chi_\Lambda \ . \tag{6.84}$$

Lemma 6.4 *The complex number z is in the resolvent set of H_Λ iff*

$$g_\Lambda^{-1} \neq \langle \chi_\Lambda, R_0(z)\chi_\Lambda \rangle \ . \tag{6.85}$$

Proof: First, we are going to show that if $g_\Lambda^{-1} \neq \langle \chi_\Lambda, R_0(z)\chi_\Lambda \rangle$, then $R_\Lambda(z)$ is bounded. Our aim is to show that there exists a positive constant C such that $||R_\Lambda(z)\psi|| \leq C||\psi||$. Using the explicit formula for the regularized resolvent given by Equation (6.84) and the triangle inequality, we have

$$\begin{aligned} ||R_\Lambda(z)\psi|| &= ||R_0(z)\psi + K\langle R_0(\bar{z})\chi_\Lambda, \psi\rangle R_0(z)\chi_\Lambda|| && (6.86) \\ &\leq ||R_0(z)\psi|| + |K| \, |\langle R_0(\bar{z})\chi_\Lambda, \psi\rangle| \, ||R_0(z)\chi_\Lambda|| \ , && (6.87) \end{aligned}$$

where $K = \frac{1}{g_\Lambda^{-1} - \langle \chi_\Lambda, R_0(z)\chi_\Lambda \rangle}$. Since $R_0(z)$ is bounded by definition of resolvent and K is finite, it remains to show that $|\langle R_0(\bar{z})\chi_\Lambda, \psi\rangle|$ is finite. Using the Cauchy-Schwarz inequality (3.3), we get

$$|\langle R_0(\bar{z})\chi_\Lambda, \psi\rangle| \leq ||R_0(\bar{z})\chi_\Lambda|| \, ||\psi|| \ . \tag{6.88}$$

Since $\mathrm{Im}(z) > 0$, and H_0 is self-adjoint, $\mathrm{Im}(\bar{z}) < 0$, $\bar{z} \in \rho(H_0)$. This means that $R_0(\bar{z})$ is bounded, then $|\langle R_0(\bar{z})\chi_\Lambda, \psi\rangle|$ is finite. Hence, we find $R_\Lambda(z)$ is bounded.

Conversely, now we will show what happens when

$$\frac{1}{g_\Lambda} = \langle \chi_\Lambda, R_0(z)\chi_\Lambda \rangle \ . \tag{6.89}$$

Consider $(H_\Lambda - zI)(H_0 - zI)^{-1}\chi_\Lambda$ and note that

$$(H_\Lambda - zI)(H_0 - zI)^{-1}\chi_\Lambda = (H_0 - g_\Lambda \mathbb{P}_{\chi_\Lambda} - zI)(H_0 - zI)^{-1}\chi_\Lambda \quad (6.90)$$
$$= \chi_\Lambda - g_\Lambda \mathbb{P}_{\chi_\Lambda}(H_0 - zI)^{-1}\chi_\Lambda \, . \quad (6.91)$$

Here the projection operator $\mathbb{P}_{\chi_\Lambda}$ acts on the vector $(H_0 - zI)^{-1}\chi_\Lambda$, so we can rewrite it as:

$$(H_\Lambda - zI)(H_0 - zI)^{-1}\chi_\Lambda = \chi_\Lambda - g_\Lambda \langle \chi_\Lambda, (H_0 - zI)^{-1}\chi_\Lambda \rangle \chi_\Lambda \quad (6.92)$$
$$= (1 - g_\Lambda \langle \chi_\Lambda, (H_0 - zI)^{-1}\chi_\Lambda \rangle)\chi_\Lambda \, . \quad (6.93)$$

This means that

$$(H_\Lambda - zI)R_0(z)\chi_\Lambda = 0 \, , \quad (6.94)$$

or

$$H_\Lambda R_0(z)\chi_\Lambda = zR_0(z)\chi_\Lambda \, . \quad (6.95)$$

Hence, $R_0(z)\chi_\Lambda$ is an eigenvector of H_Λ with the eigenvalue z as long as we need to show that $R_0(z)\chi_\Lambda$ is non zero. For this, suppose to the contrary, that is,

$$R_0(z)\chi_\Lambda = 0 \, . \quad (6.96)$$

If we multiply (6.96) by $(H_0 - z)$ from left, we get

$$\underbrace{(H_0 - z)R_0(z)}_{=I}\chi_\Lambda = 0 \, . \quad (6.97)$$

This leads to $\chi_\Lambda = 0$, which is a contradiction. Hence $R_0(z)\chi_\Lambda \neq 0$ is an eigenvector. Therefore, if z is an eigenvalue of H_Λ, then $z \in \sigma(H_\Lambda)$ (see Definition 4.19). Therefore $z \notin \rho(H_\Lambda)$. Hence, the formula for the regularized resolvent (6.80) is consistent with our result. $\square$.

This lemma simply says that $\rho(H_\Lambda) = \{z \in \mathbb{C} : g_\Lambda^{-1} \neq \langle \chi_\Lambda, R_0(z)\chi_\Lambda \rangle\}$.

Let us compute the term $\langle \chi_\Lambda, R_0(z)\chi_\Lambda \rangle$ explicitly

$$\langle \chi_\Lambda, R_0(z)\chi_\Lambda \rangle = \int\limits_{|\mathbf{p}|\leq\Lambda} \frac{1}{\mathbf{p}^2 - z} \frac{d\mathbf{p}}{(2\pi)^2} = \frac{1}{(2\pi)^2} \int_0^{2\pi} \int_0^{\Lambda} \frac{p}{p^2 - z} \, dp \, d\theta \quad (6.98)$$

$$= \frac{1}{4\pi} \log(\frac{|\Lambda^2 - z|}{|z|}) , \quad (6.99)$$

which is divergent as $\Lambda \to \infty$.

In the next step, we will choose $g_\Lambda(\mu)$ in such a way that the result is finite after removing the cut-off parameter Λ. This is motivated by the so-called renormalization idea, originally introduced in the Quantum Field Theory (Maggiore, 2005). For this reason, we choose

$$g_\Lambda := g_\Lambda(\mu) = \left(\int\limits_{|\mathbf{p}|\leq\Lambda} \frac{1}{\mathbf{p}^2 + \mu^2} \frac{d\mathbf{p}}{(2\pi)^2} \right)^{-1} , \quad (6.100)$$

where $\mu > 0$ is some parameter, fixed by experiment (once this is fixed by the experiment, the prediction of the theory can be tested by computing other observables, such as scattering cross section). Then, for z is real and negative we obtain the following expression

$$\begin{aligned} g_\Lambda^{-1}(\mu) - \langle \chi_\Lambda, R_0(z)\chi_\Lambda \rangle &= \int\limits_{|\mathbf{p}|\leq\Lambda} \frac{1}{\mathbf{p}^2 + \mu^2} \frac{d\mathbf{p}}{(2\pi)^2} - \int\limits_{|\mathbf{p}|\leq\Lambda} \frac{1}{\mathbf{p}^2 - z} \frac{d\mathbf{p}}{(2\pi)^2} \\ &= \int_0^{\Lambda} \int_0^{2\pi} \left(\frac{p}{\mathbf{p}^2 + \mu^2} - \frac{p}{\mathbf{p}^2 - z} \right) \frac{d\theta dp}{(2\pi)^2} \\ &= \frac{2\pi}{(2\pi)^2} \left(\int_0^{\Lambda} \frac{p}{\mathbf{p}^2 + \mu^2} - \frac{p}{\mathbf{p}^2 - z} \, dp \right) \\ &= \frac{1}{4\pi} \Big[\left(\log\left(\Lambda^2 + \mu^2\right) - \log\left(\mu^2\right) \right) \\ &\quad - \left(\log\left(|\Lambda^2 - z|\right) - \log\left(|z|\right) \right) \Big] \\ &= \frac{1}{4\pi} \log\left(\frac{\Lambda^2 + \mu^2}{|\Lambda^2 - z|} \right) + \frac{1}{4\pi} \log\left(\frac{|z|}{\mu^2} \right) . \end{aligned}$$

Note that the first term vanishes as Λ goes to infinity and we get $\frac{1}{4\pi} \log\left(\frac{|z|}{\mu^2} \right)$. For simplicity, we define a new function

$$\Phi_\Lambda(a,b) := \int\limits_{|\mathbf{p}|\leq\Lambda} (\mathbf{p}^2+a)^{-1}\, \frac{d\mathbf{p}}{(2\pi)^2} - \int\limits_{|\mathbf{p}|\leq\Lambda} (\mathbf{p}^2+b)^{-1}\, \frac{d\mathbf{p}}{(2\pi)^2} \;, \tag{6.101}$$

then the resolvent can be expressed in terms if Φ_Λ

$$R_\Lambda(z) = R_0(z) + \Phi_\Lambda^{-1}(\mu^2, -z)\langle R_0(\bar{z})\chi_\Lambda, .\rangle R_0(z)\chi_\Lambda \;, \tag{6.102}$$

where

$$\lim_{\Lambda\to\infty} \Phi_\Lambda(a,b) = \frac{1}{4\pi}\log(b/a) := \Phi(a,b) \;, \tag{6.103}$$

for $a, b > 0$ and $\Phi_\Lambda(\mu^2, -z)$ should be considered as the analytic continuation of the function $\Phi_\Lambda(a,b)$ defined for real positive values of a and b.

Theorem 6.5

$$\lim_{\Lambda\to\infty} R_\Lambda(z) = R(z) \;, \tag{6.104}$$

for real and negative z with $z \neq -\mu^2$ in the strong sense, where

$$R(z) = R_0(z) + \Phi^{-1}(\mu^2, -z)\mathbb{P}_{\Omega_z} = R_0(z) + \frac{4\pi}{\log(-z/\mu^2)}\mathbb{P}_{\Omega_z} \;. \tag{6.105}$$

Here $\Omega_z(\mathbf{p}) \in L^2(\mathbb{R}^2)$ is defined by

$$\Omega_z(\mathbf{p}) = \frac{1}{\mathbf{p}^2 - z} \;. \tag{6.106}$$

Proof: Suppose z is real number and not in $\{-\mu^2\} \cup [0, \infty)$, then $\bar{z} = z$ and

$$\begin{aligned} R_\Lambda(z) &= R_0(z) + \Phi_\Lambda^{-1}(\mu^2, -z)\langle R_0(\bar{z})\chi_\Lambda, .\rangle R_0(z)\chi_\Lambda && (6.107) \\ &= R_0(z) + \Phi_\Lambda^{-1}(\mu^2, -z)\langle R_0(z)\chi_\Lambda, .\rangle R_0(z)\chi_\Lambda && (6.108) \\ &= R_0(z) + \Phi_\Lambda^{-1}(\mu^2, -z)\mathbb{P}_{R_0(z)\chi_\Lambda} . && (6.109) \end{aligned}$$

Moreover,

$$\lim_{\Lambda\to\infty} \Phi_\Lambda(\mu^2, -z) = \Phi(\mu^2, -z) = \frac{1}{4\pi} \log\left(-\frac{z}{\mu^2}\right) . \quad (6.110)$$

For $\psi \in \mathcal{H}$, we have

$$||[R_\Lambda(z) - R(z)]\,\psi|| = \left|\left|\left[\Phi_\Lambda^{-1}\left(\mu^2, -z\right)\mathbb{P}_{R_0(z)\chi_\Lambda} - \Phi^{-1}\left(\mu^2, -z\right)\mathbb{P}_{\Omega_z}\right]\psi\right|\right| . \quad (6.111)$$

Using $((H_0 - zI)\psi)(\mathbf{p}) = (p^2 - z)\psi(\mathbf{p})$, we get $\psi(\mathbf{p}) = ((H_0 - zI)^{-1}(p^2 - z)\psi)(\mathbf{p})$. This means that $((R_0(z)\psi)(\mathbf{p}) = (H_0 - zI)^{-1}\psi)(\mathbf{p}) = \frac{\psi(\mathbf{p})}{p^2 - z}$. Then, we can find the action of the following projection operators:

$$\begin{aligned} (\mathbb{P}_{R_0(z)\chi_\Lambda}\psi)(\mathbf{p}) &= \langle R_0(z)\chi_\Lambda, \psi\rangle (R_0(z)\chi_\Lambda)(\mathbf{p}) && (6.112) \\ &= \left(\int_{\mathbb{R}^2} R_0(\bar{z})\chi_\Lambda(\mathbf{q})\psi(\mathbf{q})\, \frac{d\mathbf{q}}{(2\pi)^2}\right) \frac{\chi_\Lambda(\mathbf{p})}{\mathbf{p}^2 - z} && (6.113) \\ &= \left(\int_{\mathbb{R}^2} \frac{\chi_\Lambda(\mathbf{q})\psi(\mathbf{q})}{\mathbf{q}^2 - z}\, \frac{d\mathbf{q}}{(2\pi)^2}\right) \frac{\chi_\Lambda(\mathbf{p})}{\mathbf{p}^2 - z} , && (6.114) \end{aligned}$$

and

$$(\mathbb{P}_{\Omega_z}\psi)(\mathbf{p}) = \langle \Omega_z, \psi\rangle \Omega_z(\mathbf{p}) = \left(\int_{\mathbb{R}^2} \frac{\psi(\mathbf{q})}{\mathbf{q}^2 - z}\, \frac{d\mathbf{q}}{(2\pi)^2}\right) \frac{1}{\mathbf{p}^2 - z} . \quad (6.115)$$

Using the Equation (6.114) and the Equation (6.115) in Equation (6.111), we get

$$\begin{aligned} &|| \left[R_\Lambda\left(z\right) - R\left(z\right)\right] \psi || \\ &= \left\| \Phi_\Lambda^{-1}(\mu^2, -z) \left(\int_{\mathbb{R}^2} \frac{\chi_\Lambda(\mathbf{q}) \psi(\mathbf{q})}{\mathbf{q}^2 - z} \frac{d\mathbf{q}}{(2\pi)^2} \right) \frac{\chi_\Lambda(\mathbf{p})}{\mathbf{p}^2 - z} \right. \\ &\qquad \left. - \Phi^{-1}(\mu^2, -z) \left(\int_{\mathbb{R}^2} \frac{\psi(\mathbf{q})}{\mathbf{q}^2 - z} \frac{d\mathbf{q}}{(2\pi)^2} \right) \frac{1}{\mathbf{p}^2 - z} \right\| . \end{aligned}$$

Adding and subtracting the term $\frac{\Phi_\Lambda^{-1}(\mu^2,-z)}{\mathbf{p}^2-z} \int_{\mathbb{R}^2} \frac{\psi(\mathbf{q})}{\mathbf{q}^2-z} \frac{d\mathbf{q}}{(2\pi)^2}$ inside the above norm, we obtain

$$\begin{aligned} || \left[R_\Lambda\left(z\right) - R\left(z\right)\right] \psi || = &\left\| \Phi_\Lambda^{-1}(\mu^2, -z) \left[\int_{\mathbb{R}^2} \frac{\psi(\mathbf{q})}{\mathbf{q}^2 - z} \left(\frac{\chi_\Lambda(\mathbf{q}) \chi_\Lambda(\mathbf{p})}{\mathbf{p}^2 - z} - \frac{1}{\mathbf{p}^2 - z} \right) \frac{d\mathbf{q}}{(2\pi)^2} \right] \right. \\ &\left. + \int_{\mathbb{R}^2} \frac{\psi(\mathbf{q})}{\mathbf{q}^2 - z} \frac{d\mathbf{q}}{(2\pi)^2} \frac{1}{\mathbf{p}^2 - z} \left[\Phi_\Lambda^{-1}(\mu^2, -z) - \Phi^{-1}(\mu^2, -z) \right] \right\| . \end{aligned}$$

Using the triangle inequality, we have

$$\begin{aligned} &|| \big[R_\Lambda\big(z\big) - R\big(z\big)\big] \psi || \\ &\qquad \leq \quad \left| \Phi_\Lambda^{-1}(\mu^2, -z) \right| \left\| \int_{\mathbb{R}^2} \frac{\psi(\mathbf{q})}{(\mathbf{q}^2 - z)(\mathbf{p}^2 - z)} \left(\chi_\Lambda(\mathbf{q}) \chi_\Lambda(\mathbf{p}) - 1 \right) \frac{d\mathbf{q}}{(2\pi)^2} \right\| \\ &\qquad + \left| \Phi_\Lambda^{-1}\left(\mu^2, -z\right) - \Phi^{-1}\left(\mu^2, -z\right) \right| \left\| \left(\int_{\mathbb{R}^2} \frac{\psi(\mathbf{q})}{\mathbf{q}^2 - z} \frac{d\mathbf{q}}{(2\pi)^2} \right) \frac{1}{\mathbf{p}^2 - z} \right\| . \end{aligned}$$

Due to the continuity of the norm, the first term is going to zero as $\Lambda \to \infty$. For the second term, it is easy to show that

$$\int_{\mathbb{R}^2} \frac{\psi(\mathbf{q})}{q^2 - z} \frac{d\mathbf{q}}{(2\pi)^2} \tag{6.116}$$

is finite. Using the Cauchy-Schwarz inequality (3.3), we have

$$\int_{\mathbb{R}^2} \frac{\psi(\mathbf{q})}{q^2 - z} \frac{d\mathbf{q}}{(2\pi)^2} \leq \left(\int_{\mathbb{R}^2} |\psi(\mathbf{q})|^2 \frac{d\mathbf{q}}{(2\pi)^2} \right)^{1/2} \left(\int_{\mathbb{R}^2} \frac{1}{q^2 - z} \frac{d\mathbf{q}}{(2\pi)^2} \right)^{1/2} . \tag{6.117}$$

Moreover,

$$\lim_{\Lambda \to \infty} \left| \Phi_{\Lambda}^{-1}(\mu^2, -z) - \Phi^{-1}(\mu^2, -z) \right| = 0 . \tag{6.118}$$

So we end up with

$$R(z) = \lim_{\Lambda \to \infty} R_{\Lambda}(z) . \tag{6.119}$$

in the strong sense for real z and not in $\{-\mu^2\} \cup [0, \infty)$. □

Theorem 6.6 *$R(z)$ has an inverse for real z and not in $\{-\mu^2\} \cup [0, \infty)$.*

Proof:

In order to show

$$Ker R(z) = \{0\} , \tag{6.120}$$

for the above restricted values of z it would be sufficient to find a dense subset of the domain of H_{Λ}, i.e.,

$$D \subseteq D(H_{\Lambda}) = D(H_0) \tag{6.121}$$

such that the following limit exists:

$$\lim_{\Lambda \to \infty} (H_{\Lambda} - zI)\eta , \tag{6.122}$$

for $\eta \in D$. Let us call this limit as η^*. In this case, if $R(z)\psi = 0$ we then have

$$\langle \eta, \psi \rangle = \lim_{\Lambda \to \infty} \langle (H_{\Lambda} - z)\eta, R_{\Lambda}(z)\psi \rangle = \langle \eta^*, R(z)\psi \rangle = 0 , \tag{6.123}$$

for all $\eta \in D$ (dense in $D(H_{\Lambda})$) so that $\psi = 0$. Here we have used the fact that z is real and the inner product is continuous.

We now consider the set of functions $u \in S(\mathbb{R}^2)$-Schwartz space- so that their inverse Fourier transform $\mathcal{F}^{-1}$ is in $C_0^{\infty}(\mathbb{R}^2 \setminus \{0\})$-the set of smooth functions vanishing at zero and outside of some compact region. For D, we choose such functions, so that we have

$$(H_\Lambda u)(\mathbf{p}) = \mathbf{p}^2 u(\mathbf{p}) - g_\Lambda \chi_\Lambda(\mathbf{p}) \int_{\mathbb{R}^2} \chi_\Lambda(\mathbf{q}) u(\mathbf{q}) \, \frac{d\mathbf{q}}{(2\pi)^2} \; . \tag{6.124}$$

We will show that

$$||H_\Lambda u - H_0 u|| \to 0 \; , \tag{6.125}$$

as $\Lambda \to \infty$. First, it is easy to see

$$||\chi_\Lambda|| = \left[\int_{\mathbb{R}^2} |\chi_\Lambda(\mathbf{q})|^2 \; \frac{d\mathbf{q}}{(2\pi)^2} \right]^{1/2} = \left[\frac{1}{2\pi} \int_0^\Lambda p \; dp \right]^{1/2} = \frac{\Lambda}{\sqrt{4\pi}} \; . \tag{6.126}$$

Then, we get

$$\begin{aligned} ||(H_\Lambda - H_0)u|| &= \left(\int_{\mathbb{R}^2} \left[|g_\Lambda|^2 |\chi_\Lambda(\mathbf{p})|^2 \left| \int_{\mathbb{R}^2} \chi_\Lambda(\mathbf{q}) \; u(\mathbf{q}) \; \frac{d\mathbf{q}}{(2\pi)^2} \right|^2 \right] \; \frac{d\mathbf{p}}{(2\pi)^2} \right)^{1/2} && (6.127) \\ &= |g_\Lambda| \underbrace{||\chi_\Lambda||}_{\frac{\Lambda}{\sqrt{4\pi}}} \left| \int_{\mathbb{R}^2} \chi_\Lambda(\mathbf{q}) \; u(\mathbf{q}) \; \frac{d\mathbf{q}}{(2\pi)^2} \right| \; . && (6.128) \end{aligned}$$

Since $g_\Lambda(\mu)$ converges logarithmically to zero, i.e.,

$$\lim_{\Lambda \to \infty} g_\Lambda(\mu) = \lim_{\Lambda \to \infty} \frac{4\pi}{\log\left(\frac{\Lambda^2 + \mu^2}{\mu^2} \right)} = 0 \; , \tag{6.129}$$

it is sufficient to show that

$$\int_{\mathbb{R}^2} \chi_\Lambda(\mathbf{p}) \; u(\mathbf{p}) \; \frac{d\mathbf{p}}{(2\pi)^2} = O(\Lambda^{-1}) \tag{6.130}$$

to guarantee that

$$\lim_{\Lambda \to \infty} ||H_\Lambda u - H_0 u|| = 0 \; . \tag{6.131}$$

If we apply the Cauchy-Schwarz inequality (3.3) to

$$\int_{\mathbb{R}^2} \chi_\Lambda(\mathbf{q})\, u(\mathbf{q})\, \frac{d\mathbf{q}}{(2\pi)^2} \;, \tag{6.132}$$

we would get terms of the order Λ, namely $O(\Lambda)$. So we should find a smarter way.

In order to show this technical part, we first approximate the sharp (non-smooth) cut-off function $\chi_\Lambda(\mathbf{q}) = \chi_1(\mathbf{q}/\Lambda)$ by some smooth function through the following convolution

$$\chi^*_\Lambda(\mathbf{q}) = \chi^*(\mathbf{q}/\Lambda) = \int_{\mathbb{R}^2} \phi_\delta(\mathbf{q}-\mathbf{p})\, \chi_\Lambda(\mathbf{p})\, \frac{d\mathbf{p}}{(2\pi)^2} \;, \tag{6.133}$$

where

$$\phi_\delta(\mathbf{p}) = \delta^{-2}\phi(\mathbf{p}/\delta) \;, \tag{6.134}$$

is a compactly supported smooth function with support $\mathcal{B}_\delta(\mathbf{0})$ and $\lim_{\delta\to 0}\phi_\delta(\mathbf{p}) = \delta(\mathbf{p})$ in the distributional sense. This function ϕ is known as mollifier (Lieb and Loss, 2001). This replacement is known as the smooth approximation to the characteristic function of unit disc $\chi_\Lambda(\mathbf{p})$. One can show that the difference is $O(\Lambda^{-n})$ for any n if δ is chosen properly, depending on Λ (see for instance (Dimock and Rajeev, 2004)). Using the triangle inequality, we have

$$\begin{aligned} \left| \int_{\mathbb{R}^2} \chi_\Lambda(\mathbf{q})\, u(\mathbf{q})\, \frac{d\mathbf{q}}{(2\pi)^2} \right| &= \left| \int_{\mathbb{R}^2} \left[\chi_\Lambda(\mathbf{q}) - \chi^*_\Lambda(\mathbf{q}) + \chi^*_\Lambda(\mathbf{q})\right] u(\mathbf{q})\, \frac{d\mathbf{q}}{(2\pi)^2} \right| \\ &\leq \int_{\mathbb{R}^2} \left|\chi_\Lambda(\mathbf{q}) - \chi^*_\Lambda(\mathbf{q})\right| u(\mathbf{q})\, \frac{d\mathbf{q}}{(2\pi)^2} + \left| \int_{\mathbb{R}^2} \chi^*_\Lambda(\mathbf{q})\, u(\mathbf{q})\, \frac{d\mathbf{q}}{(2\pi)^2} \right| \;. \end{aligned}$$

Therefore, it would be sufficient to show that

$$\int_{\mathbb{R}^2} \chi^*_\Lambda(\mathbf{q})\, u(\mathbf{q})\, \frac{d\mathbf{q}}{(2\pi)^2} = O(\Lambda^{-1}) \;. \tag{6.135}$$

Since $(\mathcal{F}^{-1}u)(\mathbf{x}) = u(\mathbf{x}) \in C_0^\infty(\mathbb{R}^2 \setminus \{0\})$ we have

$$v(\mathbf{x}) = |\mathbf{x}|^{-2} u(\mathbf{x}) \tag{6.136}$$

in the same space so that

$$u(\mathbf{p}) = -\Delta_{\mathbf{p}} v(\mathbf{p}) \;, \tag{6.137}$$

for some $v \in S(\mathbb{R}^2)$.

Using the integration by parts twice (or Green's identity) and using the properties of the function v, we get

$$\int_{\mathbb{R}^2} \chi_\Lambda^*(\mathbf{q}) u(\mathbf{q}) \, \frac{d\mathbf{q}}{(2\pi)^2} = \int_{\mathbb{R}^2} \chi_\Lambda^*(\mathbf{q}) (-\Delta_{\mathbf{q}} v(\mathbf{q})) \, \frac{d\mathbf{q}}{(2\pi)^2} \tag{6.138}$$

$$= \int_{\mathbb{R}^2} (-\Delta_{\mathbf{q}} \chi_\Lambda^*(\mathbf{q})) \, v(\mathbf{q}) \, \frac{d\mathbf{q}}{(2\pi)^2} \;. \tag{6.139}$$

Using the chain rule, it is easily seen that

$$-\Delta_{\mathbf{q}} \chi_\Lambda^*(\mathbf{q}) = -\Delta_{\mathbf{q}} \chi^*(\mathbf{q}/\Lambda) = O(\Lambda^{-2}) \;. \tag{6.140}$$

Since $v(\mathbf{q})$ is rapidly decreasing, we obtain

$$\int_{\mathbb{R}^2} \chi_\Lambda^*(\mathbf{q}) \, u(\mathbf{q}) \, \frac{d\mathbf{q}}{(2\pi)^2} = O(\Lambda^{-2}) \;. \tag{6.141}$$

where we have used the Equation (6.139). $\square$

Once we have shown the above result, the next question one may ask whether we can extend the above statements valid for the restricted values of z onto some subset of the complex plane. Moreover, we must also ask whether there exists a self-adjoint operator associated with the resolvent formula that we have obtained. This will be the topic of the next section:

6.4. Existence of Self-adjoint Operator for the Model

One natural way to define the notion of convergence for the sequence $T_m \to T$ of unbounded operators is given through the certain bounded functions of them:

Definition 6.7 *Let* H_m , $m = 1, 2, 3, \ldots$ *and* H *be a self-adjoint operators.* H_m *is said to converge to* H *in the strong resolvent sense if* $R_z(H_m) \to R_z(H)$ *strongly for all* z *with* $\mathrm{Im}(z) \neq 0$.

Theorem 6.8 (Trotter-Kato Theorem) *Let* H_m *be a sequence of self-adjoint operators. Suppose that there exist complex numbers,* λ_0 *in the upper-half plane and* μ_0 *in the lower half-plane, so that*

$$\lim_{m\to\infty} ||R_{\lambda_0}(H_m)\varphi - T_{\lambda_0}\varphi|| = 0 , \tag{6.142}$$

$$\lim_{m\to\infty} ||R_{\mu_0}(H_m)\varphi - T_{\mu_0}\varphi|| = 0 , \tag{6.143}$$

for each $\varphi \in \mathcal{H}$. *In addition, suppose that one of the limiting operators,* T_{λ_0} *or* T_{μ_0}, *has a dense range. Then there exists a self-adjoint operator* T *so that* $H_m \to T$ *in the strong resolvent sense.*

Proof: Since H_m is self-adjoint for each m, from the self-adjoint criteria (Theorem 4.20) we must have

$$Ran(H_m \pm iI) = \mathcal{H} , \tag{6.144}$$

for each m. Let λ_0 be a complex number in the upper half plane. Then, by Theorem 4.22

$$Ran(H_m - \lambda_0 I) = \mathcal{H} , \tag{6.145}$$

and $H_m - \lambda_0 I$ is invertible and satisfies the inequality (4.48), i.e.,

$$||R_{\lambda_0}(H_m)|| = ||(H_m - \lambda_0 I)^{-1}|| \leq |\,\mathrm{Im}(\lambda_0)|^{-1} . \tag{6.146}$$

Moreover, using this inequality (6.146) we can find an upper bound for the norm of the limiting operator T_{λ_0}

$$\begin{aligned} ||T_{\lambda_0}|| &= \sup_{\varphi} \frac{||T_{\lambda_0}\varphi||}{||\varphi||} && (6.147)\\ &= \sup_{\varphi} \frac{||T_{\lambda_0}\varphi + R_{\lambda_0}(H_m)\varphi - R_{\lambda_0}(H_m)\varphi||}{||\varphi||} && (6.148)\\ &\leq \sup_{\varphi} \frac{||T_{\lambda_0}\varphi - R_{\lambda_0}(H_m)\varphi||}{||\varphi||} + \sup_{\varphi} \frac{||R_{\lambda_0}(H_m)\varphi||}{||\varphi||} && (6.149)\\ &\leq \sup_{\varphi} \frac{||T_{\lambda_0}\varphi - R_{\lambda_0}(H_m)\varphi||}{||\varphi||} + ||R_{\lambda_0}(H_m)|| && (6.150)\\ &\leq \sup_{\varphi} \frac{||T_{\lambda_0}\varphi - R_{\lambda_0}(H_m)\varphi||}{||\varphi||} + |\operatorname{Im}(\lambda_0)|^{-1} . && (6.151) \end{aligned}$$

As $m \to \infty$ we get

$$||T_{\lambda_0}|| \leq |\operatorname{Im}(\lambda_0)|^{-1} . \tag{6.152}$$

Using this fact, we can construct a new bounded operator by Proposition 3.47 as follows:

$$T_\lambda := \sum_{n=0}^{\infty} (\lambda - \lambda_0)^n T_{\lambda_0}^{n+1} , \tag{6.153}$$

where the radius of convergence is given by $|\lambda - \lambda_0| < |\operatorname{Im}(\lambda_0)|$. The reason for this is based on the following observation: $|\lambda - \lambda_0| ||T_{\lambda_0}|| < |\lambda - \lambda_0| |\operatorname{Im}(\lambda_0)|^{-1}$. If we impose $|\lambda - \lambda_0| |\operatorname{Im}(\lambda_0)|^{-1} < 1$, then the above series converges in Banach space, inside this radius of convergence (by Proposition 3.47).

Similarly, by Proposition 4.17, we can define $R_\lambda(H_m)$ from $R_{\lambda_0}(H_m)$ as follows

$$R_\lambda(H_m) := \sum_{n=0}^{\infty} (\lambda - \lambda_0)^n R_{\lambda_0}(H_m)^{n+1} , \tag{6.154}$$

where $\lambda_0 \in \rho(H_m)$ and $\lambda \in \rho(H_m)$ with $|\lambda - \lambda_0| < |\operatorname{Im}(\lambda_0)|$. Note that $R_\lambda(H_m)$ is an operator-valued analytic function on its resolvent set $\rho(H_m)$ for each m.

Using triangle inequality we have

$$\begin{aligned}||(R_\lambda(H_m)-T_\lambda)\varphi|| &= \left|\left|\left(\sum_{n=0}^{\infty}(\lambda-\lambda_0)^n R_{\lambda_0}^{n+1}(H_m)-\sum_{n=0}^{\infty}(\lambda-\lambda_0)^n T_{\lambda_0}^{n+1}\right)\varphi\right|\right| \\ &= \left|\left|\left(\sum_{n=0}^{\infty}(\lambda-\lambda_0)^n\left(R_{\lambda_0}^{n+1}(H_m)-T_{\lambda_0}^{n+1}\right)\right)\varphi\right|\right| \\ &\leq \sum_{n=0}^{\infty}|\lambda-\lambda_0|^n\left|\left|\left(R_{\lambda_0}^{n+1}(H_m)-T_{\lambda_0}^{n+1}\right)\varphi\right|\right| .\end{aligned}$$

Finally, we use proof by induction method to show $\left|\left|\left(R_{\lambda_0}^{n+1}(H_m)-T_{\lambda_0}^{n+1}\right)\varphi\right|\right| \to 0$ as $m\to\infty$ for each $n\in\mathbb{N}$ by using $||R_{\lambda_0}(H_m)-T_{\lambda_0}||\to 0$ as follows:

Suppose $n=1$, then it is clear from the main assumption

$$\left|\left|\left(R_{\lambda_0}(H_m)-T_{\lambda_0}\right)\varphi\right|\right| \to 0 ,$$

as $m\to\infty$. By induction assumption, we have

$$\left|\left|\left(R_{\lambda_0}^{k+1}(H_m)-T_{\lambda_0}^{k+1}\right)\varphi\right|\right| \to 0 ,$$

as $m\to\infty$ for $n=k$. Then using triangle inequality, we get

$$\begin{aligned}&\left|\left|\left(R_{\lambda_0}^{k+2}(H_m)-T_{\lambda_0}^{k+2}\right)\varphi\right|\right| \\ &\qquad = \left|\left|\left(R_{\lambda_0}^{k+2}(H_m)+R_{\lambda_0}^{k+1}(H_m)T_{\lambda_0}-R_{\lambda_0}^{k+1}T_{\lambda_0}-T_{\lambda_0}^{k+2}\right)\varphi\right|\right| \\ &\qquad \leq \left|\left|R_{\lambda_0}^{k+1}(H_m)\right|\right|\,\left|\left|\left(R_{\lambda_0}(H_m)-T_{\lambda_0}\right)\varphi\right|\right| \\ &\qquad\qquad\qquad + \left|\left|\left(R_{\lambda_0}^{k+1}(H_m)-T_{\lambda_0}^{k+1}\right)\right|\right|\,\left|\left|T_{\lambda_0}\varphi\right|\right| .\end{aligned}$$

Since $R_{\lambda_0}(H_m)$ and T_{λ_0} are bounded, induction hypothesis implies that

$$\left|\left|\left(R_{\lambda_0}^{k+2}(H_m)-T_{\lambda_0}^{k+2}\right)\varphi\right|\right| \to 0 , \tag{6.155}$$

as $m \to \infty$. Therefore $|| \left(R_\lambda(H_m) - T_\lambda\right) \varphi|| \to 0$ as $m \to \infty$ in the same circle $|\lambda - \lambda_0| \leq |\operatorname{Im}(\lambda_0)|$.

By continuing in this way one can define an analytic operator valued function T_λ in

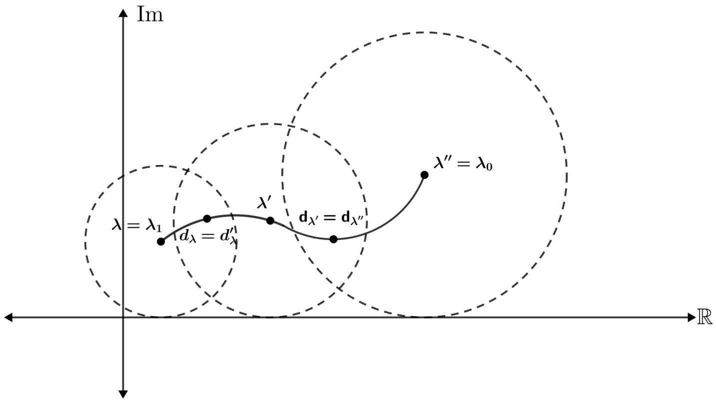

Figure 6.1. Analytic Continuation

the half plane containing the point λ_0, which is the strong limit of $R_\lambda(H_m)$. Thanks to the simply connectedness of the complex upper half plane, the determination of T_λ at λ is independent of the path starting from the point λ_0 to the point λ (Greene and Krantz, 2006). The same argument applies for the lower half plane containing the point μ_0. We thus get

$$T_\lambda \varphi = \lim_{m\to\infty} R_\lambda(H_m)\varphi \; . \tag{6.156}$$

Since $R_\lambda(H_m)$ satisfies the first resolvent identity

$$R_{\lambda_1}(H_m) - R_{\lambda_2}(H_m) = (\lambda_1 - \lambda_2) R_{\lambda_1}(H_m) R_{\lambda_2}(H_m) \; , \tag{6.157}$$

for all λ with $\operatorname{Im}(\lambda) \neq 0$, we can show that T_λ must also satisfy the first resolvent identity. This can be shown as follows. An easy computation shows that

$$\begin{aligned} ||R_{\lambda_1}(H_m)\varphi - R_{\lambda_2}(H_m)\varphi - (T_{\lambda_1}\varphi - T_{\lambda_2}\varphi)|| \;&\leq\; \underbrace{||R_{\lambda_1}(H_m)\varphi - T_{\lambda_1}\varphi||}_{\to 0 \text{ as } m\to\infty} \\ &+\; \underbrace{||R_{\lambda_2}(H_m)\varphi - T_{\lambda_2}\varphi||}_{\to 0 \text{ as } m\to\infty} \; . \end{aligned}$$

Therefore,

$$||R_{\lambda_1}(H_m)\varphi - R_{\lambda_2}(H_m)\varphi - (T_{\lambda_1}\varphi - T_{\lambda_2}\varphi)|| \to 0 \ , \tag{6.158}$$

as $m \to \infty$. On the other hand

$$\begin{aligned} ||\big[(\lambda_1 - \lambda_2)R_{\lambda_1}(H_m)R_{\lambda_2}(H_m) \ &- \ (\lambda_1 - \lambda_2)T_{\lambda_1}T_{\lambda_2}\big]\varphi|| \\ &= \ |\lambda_1 - \lambda_2|||\big[R_{\lambda_1}(H_m)R_{\lambda_2}(H_m) - T_{\lambda_1}T_{\lambda_2}\big]\varphi|| \ . \end{aligned}$$

Adding and subtracting $R_{\lambda_1}(H_m)T_{\lambda_2}$ and using triangle inequality we get

$$\begin{aligned} ||\left[R_{\lambda_1}(H_m)R_{\lambda_2}(H_m) - T_{\lambda_1}T_{\lambda_2}\right]\varphi|| \ &\leq \ \underbrace{||R_{\lambda_1}(H_m)\left(R_{\lambda_2}(H_m) - T_{\lambda_2}\right)\varphi||}_{=||R_{\lambda_1}(H_m)||\ ||\left(R_{\lambda_2}(H_m)-T_{\lambda_2}\right)\varphi||} \\ &+ \ \underbrace{||\left(R_{\lambda_1}(H_m) - T_{\lambda_1}\right)T_{\lambda_2}\varphi||}_{=||R_{\lambda_1}(H_m)-T_{\lambda_1}||\ ||T_{\lambda_2}\varphi||} \ . \end{aligned}$$

Since $||\left(R_{\lambda_2}(H_m) - T_{\lambda_2}\right)\varphi||$ and $||R_{\lambda_1}(H_m) - T_{\lambda_1}||$ goes to zero as m goes to infinity, we get

$$||\left[(\lambda_1 - \lambda_2)R_{\lambda_1}(H_m)R_{\lambda_2}(H_m) - (\lambda_1 - \lambda_2)T_{\lambda_1}T_{\lambda_2}\right]\varphi|| \to 0 \ , \tag{6.159}$$

as $m \to \infty$. Hence by (6.157), (6.158) and (6.159) and uniqueness of limit we have

$$T_{\lambda_1} - T_{\lambda_2} = (\lambda_1 - \lambda_2)T_{\lambda_1}T_{\lambda_2} \ . \tag{6.160}$$

In order to show $T_\lambda^* = T_{\bar{\lambda}}$, we first show $R_\lambda^*(H_m) = R_{\bar{\lambda}}(H_m)$. Since H_m is self-adjoint and its range is dense, the Theorem 3.59 implies that

$$\begin{aligned} (R_\lambda(H_m))^* \ &= \ \left((H_m - \lambda I)^{-1}\right)^* && (6.161) \\ &= \ ((H_m - \lambda I)^*)^{-1} && (6.162) \\ &= \ \left((H_m^* - \bar{\lambda} I\right)^{-1} && (6.163) \\ &= \ \left((H_m - \bar{\lambda} I\right)^{-1} && (6.164) \\ &= \ R_{\bar{\lambda}}(H_m) \ , && (6.165) \end{aligned}$$

for each m.

Equation (6.156) says that $R_\lambda(T_n)$ converges strongly to T_λ, i.e.,

$$\text{s-}\lim_{m\to\infty} R_\lambda(H_m) = T_\lambda \ . \tag{6.166}$$

Since strong convergence implies weak convergence and $R^*_\lambda(H_m) = R_{\bar\lambda}(H_m)$, we have

$$\begin{aligned} \lim_{m\to\infty} \langle \psi, R_\lambda(H_m)\varphi\rangle &= \lim_{m\to\infty} \langle R^*_\lambda(H_m)\psi, \varphi\rangle & (6.167)\\ &= \lim_{m\to\infty} \langle R_{\bar\lambda}(H_m)\psi, \varphi\rangle = \langle T_{\bar\lambda}\psi, \varphi\rangle \ . & (6.168)\end{aligned}$$

On the other hand, we also have

$$\lim_{m\to\infty} \langle \psi, R_\lambda(H_m)\varphi\rangle = \langle \psi, T_\lambda\varphi\rangle = \langle T^*_\lambda\psi, \varphi\rangle \ . \tag{6.169}$$

Comparing the two results (6.168) and (6.169), we get

$$\langle (T_{\bar\lambda} - T^*_\lambda)\psi, \varphi\rangle = 0 \ , \tag{6.170}$$

for all φ, ψ. Since φ are dense in $\mathcal{H}$ we obtain

$$T^*_\lambda = T_{\bar\lambda} \ . \tag{6.171}$$

It follows from the first resolvent formula $T_{\lambda_1} - T_{\lambda_2} = (\lambda_1 - \lambda_2)T_{\lambda_1}T_{\lambda_2}$ and the commutativity $T_{\lambda_1}T_{\lambda_2} = T_{\lambda_2}T_{\lambda_1}$ (corollary of the first resolvent formula) that $Ran(T_\lambda)$ is independent of λ. This can be seen as follows. Let $\psi \in Ran(T_{\lambda_1})$, that is $\psi = T_{\lambda_1}\varphi$, where $\varphi \in D(T_{\lambda_1})$. Then, the first resolvent formula and the commutativity implies that

$$\psi - T_{\lambda_2}\varphi = (\lambda_1 - \lambda_2)T_{\lambda_2}\psi \ . \tag{6.172}$$

This clearly forces us that $\psi \in Ran(T_{\lambda_2})$, implying that $Ran(T_{\lambda_1}) \subseteq Ran(T_{\lambda_2})$.

Conversely, suppose that $\psi \in Ran(T_{\lambda_2})$, that is, $\psi = T_{\lambda_2}\varphi$, where $\varphi \in D(T_{\lambda_2})$. A similar argument given above gives

$$T_{\lambda_1}\varphi - \psi = (\lambda_1 - \lambda_2)T_{\lambda_1}\psi \; . \tag{6.173}$$

In other words, we get

$$Ran(T_{\lambda_2}) \subseteq Ran(T_{\lambda_1}) \; . \tag{6.174}$$

Hence we obtain $Ran(T_{\lambda_1}) = Ran(T_{\lambda_2})$, that is range of T_λ is independent of λ.

We will call this common range as D, that is

$$T_\lambda : \mathcal{H} \to Ran(T_\lambda) = D \; . \tag{6.175}$$

By hypothesis of the theorem, $D = Ran(T_{\lambda_0}) = Ran(T_\lambda)$ is dense in $\mathcal{H}$, i.e.,

$$\overline{Ran(T_\lambda)} = \bar{D} = \mathcal{H} \; . \tag{6.176}$$

This implies that the kernel of T_λ is empty:

$$Ker(T_\lambda) = Ran(T_\lambda^*)^\perp = Ran(T_{\bar{\lambda}})^\perp = D^\perp = \{0\} \; , \tag{6.177}$$

where we have used Proposition (3.41) and the fact that $T_\lambda^* = T_{\bar{\lambda}}$. Therefore we define a candidate operator T on this domain D as follows:

$$T := \lambda I + T_\lambda^{-1} \; . \tag{6.178}$$

This operator is independent of λ with $\mathrm{Im}(\lambda) \neq 0$. To show this, suppose that

$$T' = \lambda' I + T_{\lambda'}^{-1} \; . \tag{6.179}$$

Subtracting Equation (6.179) from Equation (6.178) we get

$$T - T' = (\lambda - \lambda')I - (T_{\lambda'}^{-1} - T_{\lambda}^{-1}) \; . \tag{6.180}$$

If we multiply both sides of the first resolvent identity for T_λ

$$T_\lambda - T_{\lambda'} = (\lambda - \lambda')T_\lambda T_{\lambda'} \; , \tag{6.181}$$

by T_λ^{-1} from the left and $T_{\lambda'}^{-1}$ from the right, then we get

$$T_{\lambda'}^{-1} - T_{\lambda}^{-1} = \lambda - \lambda' \; . \tag{6.182}$$

Plugging Equation (6.182) into the Equation (6.180) we get

$$T - T' = (\lambda - \lambda')I - (\lambda - \lambda') = 0 \; . \tag{6.183}$$

This shows that the definition of T is independent of λ. Our aim is now to show that T is self-adjoint. Since it does not depend on λ we may choose $\lambda = i$ or $\lambda = -i$ without loss of generality. Then,

$$Ran(T + iI) = Ran(-i + T_{-i}^{-1} + i) = Ran(T_{-i}^{-1}) = \mathcal{H} \; . \tag{6.184}$$

Similarly,

$$Ran(T - iI) = Ran(iI + T_{i}^{-1} + iI) = Ran(T_{i}^{-1}) = \mathcal{H} \; . \tag{6.185}$$

By the self-adjoint criteria (Theorem 4.20), T is self-adjoint.

By definition of T we have

$$
\begin{aligned}
T &= \lambda I + T_\lambda^{-1} && (6.186)\\
T - \lambda I &= T_\lambda^{-1} && (6.187)\\
(T - \lambda I)^{-1} &= T_\lambda \, . && (6.188)
\end{aligned}
$$

Hence

$$
R_\lambda(T) = T_\lambda \, . \qquad (6.189)
$$

Since we already have $||R_\lambda(H_m) - T_\lambda|| \to 0$ as $m \to \infty$, it is immediately follows from the Equation (6.189) that $||R_\lambda(H_m) - R_\lambda(T)|| \to 0$ as $m \to \infty$ which means $H_m \to T$ in the strong resolvent sense. See for instance (Reed and Simon, 1972). □

Actually we shall use a different version of Trotter-Kato theorem for our purpose. But the proof is essentially the same:

Theorem 6.9 *Let Σ be a proper closed subset of $\mathbb{R}$ and let H_m be a sequence of self-adjoint operators with resolvents $R_m(z) = (H_m - zI)^{-1}$ defined for all complex $z \notin \Sigma$. Suppose that $R_m(z)$ converges strongly for some $z \notin \Sigma$ and that the limit has an inverse. Then, there exists a self-adjoint operator H with resolvent $R(z) = (H - zI)^{-1}$ such that $R_m(z)$ converges strongly to $R(z)$ for all complex $z \notin \Sigma$.*

In the original version, we have $\Sigma = \mathbb{R}$. The proof of the above version can be easily proved by following the same line of arguments.

Theorem 6.10 $\lim_{\Lambda \to \infty} R_\Lambda(z) = R(z)$ *in the strong sense for complex* $z \in \mathbb{C} \setminus \{-\mu^2\} \cup [0, \infty)$ *and there exists a self-adjoint operator* $H(\mu)$ *such that* $R(z) = (H(\mu) - zI)^{-1}$.

Proof: This is just consequence of the previous parts and Trotter-Kato theorem. □

When we compare our result with the result given in (Albeverio et al., 1988), where they examine $-\Delta$ on $L^2(\mathbb{R}^2 \setminus \{0\})$ and construct all possible self-adjoint extensions by imposing some boundary conditions at the origin on the wave function. These self-adjoint extensions are indexed by a parameter α, where $\alpha \in \mathbb{R}$. Also an explicit resolvent formula (known as also Krein's formula) is exactly consistent with the formula (6.105) as long as we impose the following condition between the self-adjoint extension parameter α and μ:

$$\frac{1}{2}\log(-k^2/\mu^2) = 2\pi\alpha - \Psi(1) + \log(k/2i) \;, \tag{6.190}$$

where Ψ is the digamma function and $k^2 = z$ with $\mathrm{Im}(k) > 0$. This implies that these results are equivalent as long as we identify the parameter μ in our formula and the self-adjoint extension parameter α through the above expression.

6.5. Bound State Spectrum

It is easy to see that the resolvent formula $R(z)$ given by (6.105) on the complex plane has a simple pole at $z = -\mu^2$, so $-\mu^2$ is the eigenvalue of $H(\mu)$, which corresponds to the bound state of the system. Let us now find the bound state wave function associated with the bound state energy $-\mu^2$ using the Riesz integral representation (Hislop and Sigal, 2012). It simply says that the contour integral of the resolvent around its simple pole gives the projection operator onto the eigenspace spanned by the bound state function ψ:

$$\mathbb{P}_\psi = \frac{1}{2\pi i}\oint_\gamma R(z)\; dz \;, \tag{6.191}$$

where γ is the closed contour around the simple pole of the resolvent $R(z)$. Here the closed contour γ is sufficiently small that it does not intersect with the continuous spectrum of the self-adjoint operator H. What we mean by the above integral representation is:

$$\langle\psi,\varphi\rangle\psi(\mathbf{p}) = \frac{1}{2\pi i}\oint_\gamma (R(z)\varphi)(\mathbf{p})\; dz \;. \tag{6.192}$$

Since the free resolvent does not contain poles ($(R(z)\varphi)(\mathbf{p}) = \frac{\varphi(\mathbf{p})}{p^2-z}$), we find the right hand side as

$$4\pi\mu^2 \langle \frac{1}{p^2+\mu^2}, \varphi \rangle \, \frac{1}{p^2+\mu^2} \ , \tag{6.193}$$

where we have used the residue theorem (Brown et al., 2009). From this result, we can read off the bound state wave function in momentum space:

$$\psi(\mathbf{p}) = 2\sqrt{\pi}\mu \, \frac{1}{p^2+\mu^2} \ . \tag{6.194}$$

The coordinate space bound state wave function with the correct normalization can be found from the inverse Fourier transformation so we get

$$\psi(\mathbf{x}) = \frac{\mu}{\sqrt{\pi}} \, K_0(\mu|\mathbf{x}|) \ , \tag{6.195}$$

where K_0 is the modified Bessel function of the third kind. Here we have used the following integral representations in evaluating the integrals in polar coordinates of the momentum space:

$$K_0(\alpha\beta) = \int_0^\infty \frac{J_0(\beta p)}{p^2+\mu^2} \, p \, dp \ , \tag{6.196}$$

$$J_0(x) = \frac{1}{2\pi} \int_0^{2\pi} e^{ix\cos\theta} \, d\theta \ , \tag{6.197}$$

where J_0 is the Bessel function of the first kind (Lebedev, 1965). It is important to notice that the coordinate wave function $\psi(\mathbf{x})$ given in (6.195) is radially symmetric. In contrast to the one-dimensional bound state wave function given in Equation (5.94), the bound state wave function in two dimensions is singular due to the asymptotic behaviour of K_0 near the origin, i.e.,

$$K_0(r) \sim -\log(r/2) + \gamma \ , \tag{6.198}$$

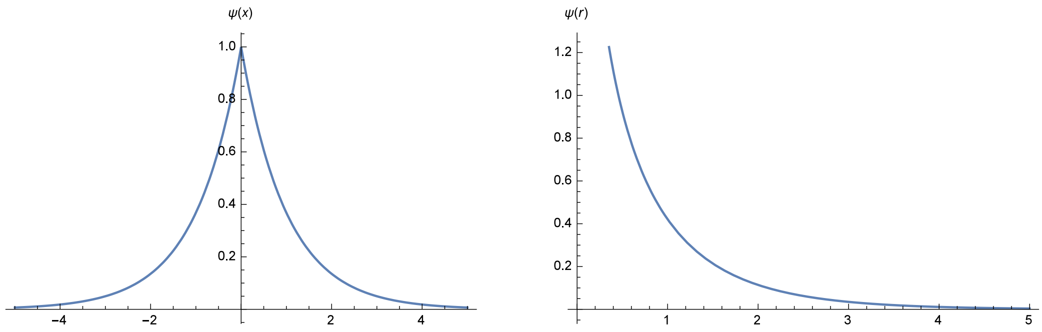

Figure 6.2. Bound State Wave functions for Dirac delta Potentials in One and Two Dimensions

as $r \to 0$. Here γ is the Euler's constant (Lebedev, 1965). The general behaviour of these wave functions are shown in Figure 6.2 Both of the bound state wave functions are decaying for large distances, as expected. The bound state wave function (5.94) in one dimension has a cusp at the origin whereas the bound state wave function (6.195) in two dimensions diverges around the origin. Nevertheless, it is easy to check that the bound state wave function (6.195) in two dimensions is square integrable, that is,

$$\int_{\mathbb{R}^2} |\psi(\mathbf{x})|^2 \, d\mathbf{x} = \int_{\mathbb{R}^2} |\psi(\mathbf{p})|^2 \, \frac{d\mathbf{p}}{(2\pi)^2} = 1 \; , \tag{6.199}$$

where we have used (6.194). It is interesting to notice that the wave function is naturally normalized so we do not need to normalize it again.

However, if we consider

$$\int_{\mathbb{R}^2} |\Delta\psi(\mathbf{x})|^2 \, d\mathbf{x} \; , \tag{6.200}$$

we see that it is divergent, i.e., $\Delta\psi \notin L^2(\mathbb{R}^2)$. This can be seen as follows. First, we go to the polar coordinates and calculate the Laplacian in polar coordinates to find

$$\int_0^\infty \int_0^{2\pi} \left| \frac{d^2\psi(r)}{dr^2} + \frac{1}{r}\frac{d\psi}{dr} \right|^2 r \, dr \, d\theta \; , \tag{6.201}$$

where we have used ψ is radially symmetric. The second derivative term can be explicitly calculated

$$2\mu^2 \int_0^\infty \left(\mu^2 K_0(\mu r) + \frac{\mu}{r} K_1(\mu r)\right)^2 r \, dr \tag{6.202}$$

by using (Lebedev, 1965)

$$\frac{d^2 K_0(\alpha r)}{dr^2} = \alpha^2 K_0(\alpha r) + \frac{\alpha}{r} K_1(\alpha r) \; . \tag{6.203}$$

The above integral (6.202) includes the following term

$$\int_0^\infty K_0(\mu r) K_1(\mu r) \, dr \; . \tag{6.204}$$

Thanks to the asymptotic expansion of the Bessel function K_0 given by (6.198) and the fact that $K_1(\alpha r) = -\alpha \frac{dK_0(\alpha r)}{dr}$, the above integral is logarithmically divergent. What this means that the functions that we have found do not lie inside the domain of the free Hamiltonian H_0 anymore. Instead, they are outside of this domain: $\Delta\psi \notin L^2(\mathbb{R}^2)$. This is completely consistent with the self-adjoint extension theory since the functions after the finding the resolvent associated with a self-adjoint operator must lie in a “bigger” space than the original domain of the free Hamiltonian.

As emphasized in the Introduction, the problem initially does not include any natural length scale. After the renormalization of the model, the model gains a length scale, namely μ^{-1}. This is known as an example of dimensional transmutation in quantum field theoretical models, in particular in gauge theories in four dimensions. Therefore, this model can be considered as a toy model for understanding such phenomena in a relatively simple way (see, for instance, (Mead and Godines, 1991; Mitra et al., 1998; Nyeo, 2000; Manuel and Tarrach, 1994; Phillips et al., 1998; Rajeev, 1999)).

One can study the spectral properties of the model once we have resolvent. This includes the study of the scattering problem, which has been discussed in (Erman, 2010; Tunalı, 2014) in detail.

This model can be directly extended to the three dimensions. The resolvent formula is exactly in the same form as in (6.105). The only difference is the form of the function ξ given in (6.103). In three dimensions, by going to spherical coordinates it is easy to show that

$$\Phi(\mu^2, -z) = \frac{1}{4\pi}\left(\sqrt{-z} - \mu\right) \ . \tag{6.205}$$

Hence, the bound state energy is still $-\mu^2$ since it is the pole of the resolvent formula or zeroes of the function ξ.

Another extension of the model is the addition of some bounded potential function V to the Dirac delta potential, and the resolvent formula is still given in the same form as in (6.105) except for the free resolvent is replaced by the resolvent associated with the operator $-\Delta + V$, see (Dimock and Rajeev, 2004) for the details.

The model can further be extended to the many bosonic particles, where the Hilbert space becomes the so-called Fock space. This is discussed in (Rajeev, 1999; Dimock and Rajeev, 2004; Erman and Turgut, 2013).

CHAPTER 7

CONCLUSION

We have reviewed the necessary background of the problem for which the model that we are interested in is formulated. These topics include some operator theory and Von Neumann's self-adjoint extension theory. Then, we heuristically present the Dirac delta potential in one dimension, as discussed in the physics literature. Moreover, the same problem has been studied from the self-adjoint extension theory.

The main subject of the thesis is a particular singular non-relativistic quantum mechanical problem, where two particles interact with each other through a singular potential, namely Dirac delta function in two dimensions. After regularizing the singular Hamiltonian and then choosing the coupling constant appropriately such that the limit of the regularized resolvent has a well-defined limit. This limit of the resolvents has been shown to be the resolvent of some self-adjoint operator. We finally discuss the bound state spectrum of the problem.

All the issues that we have discussed in this thesis are rather well-known in the literature. However, our aim is to review the subject including the necessary background of operator theory with detailed proofs so that the thesis is self-contained. Moreover, all the details of the proofs in the model that we have discussed are given in detail.

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APPENDIX A

SOME ELEMENTARY NOTIONS IN DISTRIBUTION THEORY

There are two classes of functions on which the distributions are defined, namely compactly supported smooth functions and Schwartz functions.

Definition A.1 *(Appel, 2007) The compactly supported smooth functions are the set of complex-valued infinitely differentiable functions $\varphi(\mathbf{x})$ on $\mathbb{R}^n$ (in the sense that continuous partial derivatives of all orders exist), which are compactly supported (their supports ($\operatorname{supp}(\varphi) = \overline{\{x \in D(\varphi) | \varphi(x) \neq 0\}}$ are bounded). They are usually denoted by $C_0^\infty(\mathbb{R}^n)$ or $C_c^\infty(\mathbb{R}^n)$.*

The prototype of such functions is (Kanwal, 2012)

$$\varphi(\mathbf{x}) = \begin{cases} e^{-\frac{1}{1-r^2}}, & \text{if } r < 1 \\ 0, & \text{otherwise} \end{cases} \tag{A.1}$$

where $r = |\mathbf{x}|$ and $\operatorname{supp}(\varphi(\mathbf{x})) = B(\mathbf{0}; 1)$. One can construct a sequence of $C_c^\infty(\mathbb{R}^n)$ functions by scaling the above prototype function $\varphi_m(\mathbf{x}) := c_m \varphi(\mathbf{x}/m)$, where c_m is a constant determined by normalization $\int\limits_{\mathbb{R}^n} \varphi_m(\mathbf{x})\, d\mathbf{x} = 1$. It is easy to show that $C_c^\infty(\mathbb{R}^n)$ form a vector space under point-wise addition and multiplication of functions by scalars. One can also define the continuity on this space as follows:

Definition A.2 *A sequence of functions $\{\varphi_m(\mathbf{x})\}_{m=1}^\infty \in C_c^\infty(\mathbb{R}^n)$ converges to a function $\varphi(\mathbf{x}) \in C_c^\infty(\mathbb{R}^n)$ if two following conditions met*

(i) $\operatorname{supp}(\varphi_m) \subset D$ *for all m, where D is bounded subset of $\mathbb{R}^n$.*

(ii) $\partial^{\mathbf{k}} \varphi_m \to \partial^{\mathbf{k}} \varphi$ *uniformly over $\mathbb{R}^n$ as $m \to \infty$ for all multi-indices*

$$\mathbf{k} = (k_1, k_2, \ldots, k_n)$$

with k_n's are positive integers. Here $\mathbf{x} = (x_1, x_2, \ldots, x_n)$ and

$$\partial^{\mathbf{k}} := \frac{\partial^{|\mathbf{k}|}}{\partial x_1^{k_1} \partial x_2^{k_2} \ldots \partial x_n^{k_n}} \ , \tag{A.2}$$

and $|\mathbf{k}| = k_1 + k_2 + \cdots + k_n$.

It is sometimes convenient to use the notation $D^{\mathbf{k}} = D_1^{k_1} \ldots D_n^{k_n}$, where $D_j = -i\frac{\partial}{\partial x_j}$ in Fourier analysis since the factor $(-i)$ is popping out after taking derivatives.

An another class of smooth functions with a different decaying properties are given in the following way:

Definition A.3 *The Schwartz space $S(\mathbb{R}^n)$ is the set of all complex-valued infinitely differentiable functions $\varphi(\mathbf{x})$ on $\mathbb{R}^n$, which they satisfy*

$$\sup_{\mathbf{x} \in \mathbb{R}^n} |\mathbf{x}^{\mathbf{k}} \, \partial^{\mathbf{l}} \varphi(\mathbf{x})| < \infty \ , \tag{A.3}$$

for all multi-indices $\mathbf{k}, \mathbf{l}$. Here, $\mathbf{x}^{\mathbf{l}} := x^{l_1} x^{l_2} \cdots x^{l_n}$ (see (Reed and Simon, 1972)).

In other words, the functions and their derivatives in Schwartz space vanish at infinity faster than the inverse of any polynomial (or rapidly decaying). As the name suggests, they form a vector space. A classical example of these functions is the well-known Gaussian function $e^{-|\mathbf{x}|^2/2}$. It is easy to see that $C_c^\infty(\mathbb{R}^n) \subseteq S(\mathbb{R}^n)$ since every compactly supported smooth function vanish identically outside some finite interval, whereas the above given Gaussian function only decrease rapidly at infinity.

Indeed, the Schwartz space is not a normed space, instead we have a countable family of semi-norms defined by the left hand side of the inequality (A.3)

$$||\varphi||_{\mathbf{k},\mathbf{l}} := \sup_{\mathbf{x} \in \mathbb{R}^n} |\mathbf{x}^{\mathbf{k}} \, \partial^{\mathbf{l}} \varphi(\mathbf{x})| \ . \tag{A.4}$$

This is a semi-norm on $S(\mathbb{R}^n)$ since the last property of norms is not satisfied (Chapter 3). From these collections of semi-norms one can define a metric (topology) on this space to talk about convergence and continuity (see Chapter V in (Reed and Simon, 1972) for the details).

The countable family of semi-norms allows us to define properly the convergence of the sequence of functions in $S(\mathbb{R}^n)$:

Definition A.4 *(Kanwal, 2012) Let $\{\varphi_m(\mathbf{x})\}_{m=1}^{\infty}$ be a sequence of functions in Schwartz space $S(\mathbb{R}^n)$. Then, we say that φ_m converges to φ_0 if and only if*

$$||\varphi_m - \varphi||_{\mathbf{k},\mathbf{l}} \to 0 \ , \tag{A.5}$$

as $m \to \infty$ for all $\mathbf{k}$ and $\mathbf{l}$.

Actually, Schwartz space is complete (as a metric space) - more technically it is a Freshcèt space ((Reed and Simon, 1972)). The uniqueness of the limit is guaranteed by imposing the above condition for all multi-indices. It is not hard to show that there is an equivalent useful characterization of Schwartz spaces.

Theorem A.5 *The functions $\varphi \in S(\mathbb{R}^n)$ if and only if there exists constant $C_{N,\mathbf{k}} > 0$ such that*

$$|\partial^{\mathbf{k}}\varphi(\mathbf{x})| \leq \frac{C_{N,\mathbf{k}}}{(1+|\mathbf{x}|)^N} \ , \tag{A.6}$$

for all $N \in \mathbb{N}_0 = \{0, 1, 2, \dots\}$ and $\mathbf{k}$. Here $|\mathbf{x}|$ is the Euclidean norm of the vector $\mathbf{x}$.

We now show that compactly supported smooth functions are dense in Schwartz space and then conclude that compactly supported functions are dense in $L^2(\mathbb{R}^n)$.

For this, we recall the observation that $C_c^{\infty}(\mathbb{R}^n) \subseteq S(\mathbb{R}^n)$. We choose the so-called cut-off function, namely $\rho \in C_c^{\infty}(\mathbb{R}^n)$ such that $\rho(\mathbf{x}) = 1$ if $|\mathbf{x}| \leq 1$. Let $\varphi \in S(\mathbb{R}^n)$ and define the sequence of functions $\varphi_m(\mathbf{x}) := \varphi(\mathbf{x})\rho(\mathbf{x}/m)$ where $m \in \mathbb{N}$. Then, $\varphi_m \in C_c^{\infty}(\mathbb{R}^n)$ and $\varphi(\mathbf{x}) - \varphi_m(\mathbf{x}) = 0$ when $|\mathbf{x}| \leq m$ thanks to the above chosen cut-off function. We need to show that $\varphi_m \to \varphi$ in $S(\mathbb{R}^n)$. From the definition of the semi-norm on $S(\mathbb{R}^n)$ and the definition of the cut-off function, we have

$$||\varphi - \varphi_m||_{\mathbf{k},\mathbf{l}} = \sup_{|\mathbf{x}|>m} |\mathbf{x}^{\mathbf{k}} \, \partial^{\mathbf{l}} \left(\varphi(\mathbf{x})(1 - \rho(\mathbf{x}/m))\right)| \ . \tag{A.7}$$

The partial derivatives can be computed from Leibniz rule to get

$$\partial^{\mathbf{l}}\left(\varphi(\mathbf{x})(1-\rho(\mathbf{x}/m))\right) = \sum_{\mathbf{r}\leq\mathbf{l}} \begin{pmatrix}\mathbf{l}\\ \mathbf{r}\end{pmatrix} \left(\partial^{\mathbf{l}-\mathbf{r}}\varphi(\mathbf{x})\right)\ \partial^{\mathbf{r}}\left(1-\rho(\mathbf{x}/m)\right)\ , \qquad (A.8)$$

where $\begin{pmatrix}\mathbf{l}\\ \mathbf{r}\end{pmatrix} = \frac{\mathbf{l}!}{\mathbf{r}!(\mathbf{l}-\mathbf{r})!}$, $\mathbf{l}! = l_1!\cdots l_n!$, and $\sum_{\mathbf{r}\leq\mathbf{l}} = \sum_{r_1\leq l_1}\cdots\sum_{r_n\leq l_n}$. To simplify the calculations, we can consider a typical term inside of the supremum in the equation (A.7) for ($\mathbf{r}\leq\mathbf{l}$):

$$A_{\mathbf{r}}(\mathbf{x}) := |\mathbf{x}^{\mathbf{k}}\ \left(\partial^{\mathbf{l}-\mathbf{r}}\varphi(\mathbf{x})\right)\ \partial^{\mathbf{r}}\left(1-\rho(\mathbf{x}/m)\right)|\ , \qquad (A.9)$$

for $|\mathbf{x}| > m$. For $|\mathbf{r}| > 0$, we can estimate the above expression

$$\begin{aligned}\sup_{|\mathbf{x}|>m} A_{\mathbf{r}}(\mathbf{x}) &= \sup_{|\mathbf{x}|>m} |\mathbf{x}^{\mathbf{k}}\ \left(\partial^{\mathbf{l}-\mathbf{r}}\varphi(\mathbf{x})\right)\ \frac{1}{m^{\mathbf{r}}}\partial^{\mathbf{r}}\rho(\mathbf{x}/m)| &(A.10)\\ &\leq \frac{1}{m^{\mathbf{r}}}\sup_{|\mathbf{x}|>m} |\partial^{\mathbf{r}}\rho(\mathbf{x}/m)|\ ||\varphi||_{\mathbf{k},\mathbf{l}-\mathbf{r}}\ , &(A.11)\end{aligned}$$

where we have used the chain rule and used the fact that supremum of all orders of derivative of the cut-off functions exist. Hence, $\sup_{|\mathbf{x}|>m} A_{\mathbf{r}}(\mathbf{x}) \to 0$ as $m\to\infty$.

If $\mathbf{r} = \mathbf{0}$, from the equivalent definition of the Schwartz space (Theorem A.5) and choosing $N > |\mathbf{k}|$ for every N, we obtain

$$\begin{aligned}\sup_{|\mathbf{x}|>m} A_{\mathbf{0}}(\mathbf{x}) &= \sup_{|\mathbf{x}|>m} |\mathbf{x}^{\mathbf{k}}\ \left(\partial^{\mathbf{l}}\varphi(\mathbf{x})\right)\ \left(1-\rho(\mathbf{x}/m)\right)| &(A.12)\\ &\leq \sup_{|\mathbf{x}|>m}\left(|\mathbf{x}|^{|\mathbf{k}|}\ |\partial^{\mathbf{l}}\varphi(\mathbf{x})|\right)\ \sup_{|\mathbf{x}|>m}\left(1-\rho(\mathbf{x}/m)\right)| &(A.13)\\ &\leq \sup_{|\mathbf{x}|>m}\left(1+|\mathbf{x}|\right)^{|\mathbf{k}|}\ C_{N,\mathbf{l}}(1+|\mathbf{x}|)^{-N}\ \sup_{|\mathbf{x}|>m}\left(1-\rho(\mathbf{x}/m)\right)| &(A.14)\\ &= \left(1+|m|\right)^{|\mathbf{k}|-N}\ C_{N,\mathbf{l}}\ \sup_{|\mathbf{x}|>m}\left(1-\rho(\mathbf{x}/m)\right)|\ , &(A.15)\end{aligned}$$

where we have used the fact that $|\mathbf{x}^{\mathbf{k}}| = |x_1|^{k_1}\ldots|x_n|^{k_n} \leq |x|^{k_1}\ldots|x|^{k_n} = |x|^{|\mathbf{k}|}$. This in turn implies that $\sup_{|\mathbf{x}|>m} A_{\mathbf{0}}(\mathbf{x}) \to 0$ as $m\to\infty$. Hence, we have shown that $C_c^{\infty}(\mathbb{R}^n)$ are dense in $S(\mathbb{R}^n)$.

One can also easily show the inclusion $S(\mathbb{R}^n) \subseteq L^2(\mathbf{R}^n)$. Let $\varphi \in S(\mathbb{R}^n)$ (the proof can be extended to the inclusion in $L^p(\mathbb{R}^n)$ by simply replacing the power 2 by p, where $p \in [1, \infty]$). Then,

$$\left(\int_{\mathbb{R}^n} |\varphi(\mathbf{x})|^2 \, d\mathbf{x}\right)^{1/2} = \left(\int_{\mathbb{R}^n} |\varphi(\mathbf{x})|^2 \, \frac{(1+|\mathbf{x}|)^{2(n+1)}}{(1+|\mathbf{x}|)^{2(n+1)}} \, d\mathbf{x}\right)^{1/2} \tag{A.16}$$

$$\leq \sup_{\mathbf{x}\in\mathbb{R}^n} |(1+|\mathbf{x}|)^{n+1}\varphi(\mathbf{x})| \left(\int_{\mathbb{R}^n} \frac{1}{(1+|\mathbf{x}|)^{2(n+1)}} \, d\mathbf{x}\right)^{1/2} \tag{A.17}$$

$$\leq C_{n+1,\mathbf{0}} \left(\int_{\mathbb{R}^n} \frac{1}{(1+|\mathbf{x}|)^{2(n+1)}} \, d\mathbf{x}\right)^{1/2} . \tag{A.18}$$

The convergence of the integral can easily be seen by going to spherical coordinates. Hence, this implies that $S(\mathbb{R}^n) \subseteq L^2(\mathbb{R}^n)$ so $C_c^\infty(\mathbb{R}^n)$ is dense in $L^2(\mathbb{R}^n)$ and $S(\mathbb{R}^n)$ is dense in $L^2(\mathbb{R}^n)$.

In general, test spaces are the appropriate place on which the distributions are defined, and they are in general denoted by $\mathcal{D}(\mathbb{R}^n)$. If the test space is chosen as the Schwartz space $S(\mathbb{R}^n)$, the distributions are called as tempered distributions. We first overview the distributions defined on the test space $\mathcal{D}(\mathbb{R}^n) = C_c^\infty(\mathbb{R}^n)$.

Definition A.6 *(Kanwal, 2012) A distribution $t : \mathcal{D}(\mathbb{R}^n) \to \mathbb{C}$ is a linear continuous functional acting on test functions $\mathcal{D}(\mathbb{R}^n)$ and they form a vector space denoted by $\mathcal{D}'(\mathbb{R}^n)$. Here the continuity means that $\varphi_m \to \varphi$ in $\mathcal{D}(\mathbb{R}^n)$ as $m \to \infty$ implies that $t(\varphi_m) \to t(\varphi)$ in $\mathbb{C}$ as $m \to \infty$. The most common notation for the action of distribution on test functions are given by $\langle t, \varphi\rangle$ instead of $t(\varphi)$.*

It is worth pointing out that one should be aware that the notation for the action of the distributions on the test functions is the same as our inner product notation $\langle\cdot,\cdot\rangle$ although they represent different notions.

There are usually two most important classes of distributions, namely regular distributions and singular distributions.

Definition A.7 *(Kanwal, 2012) The distributions t that can be generated by locally integrable functions f through the formula*

$$\langle t, \varphi \rangle = \int_{\mathbb{R}^n} f(\mathbf{x})\varphi(\mathbf{x})\; d\mathbf{x} = \langle t_f, \varphi \rangle \tag{A.19}$$

are called regular distributions. It is customary to abuse the notation and the right hand side is simply written $\langle f, \varphi \rangle$ instead of $\langle t_f, \varphi \rangle$.

In the above definition, one must check the linearity (trivial to see) and continuity. Using the linearity, it is easy to prove the continuity of the above functional $\langle f, \varphi \rangle$ by the below estimate

$$\langle f, \varphi_m - \varphi \rangle \leq M_m \int_D |f(\mathbf{x})|\; d\mathbf{x}\;, \tag{A.20}$$

where M_m is the maximum of $|\varphi_m - \varphi|$ and D is the common interval outside of which all the terms $|\varphi_m - \varphi|$ are zero. Since $\varphi_m \to \varphi$ in $\mathcal{D}(\mathbb{R}^n)$, above inequality implies that $\langle f, \varphi \rangle$ is a distribution. Since every piecewise continuous functions is locally integrable ($\int_{\mathbb{R}^n} f(\mathbf{x})\; d\mathbf{x}$ exists in the sense of Lebesgue for every bounded region of $\mathbb{R}^n$), Heaviside step function is a simple example for a regular distribution.

The distributions that can not be generated by a locally integrable function are called singular distributions. One of the most important singular distributions from our point of view in this thesis is the so-called Dirac delta distribution or Dirac delta function. The name Dirac refers to the physicist P. A. M. Dirac who had to use the function in a non-rigorous way since the theory of distributions had not been established yet. Actually, the non-rigorous usage of the function seems first appeared in the early part of the 19th century in the works of Poisson, Fourier, Cauchy, Kirchhoff, and Heaviside (Lützen, 2012). The reason why Dirac used this function is essentially based on the idea of unifying matrix mechanics and wave mechanics by drawing some analogies (Dirac, 1981). Let us now define it as a particular kind of distribution:

Example A.8 *(Kanwal, 2012) The Dirac delta distribution in $\mathbb{R}^n$ is defined as*

$$\langle \delta_\xi, \varphi \rangle = \varphi(\xi)\;, \tag{A.21}$$

where ξ is a fixed vector in $\mathbb{R}^n$. In particular, if $\xi = \mathbf{0}$, then we use the following notation $\langle \delta, \varphi \rangle = \varphi(\mathbf{0})$ for simplicity.

One can check that the Dirac delta distribution is indeed a distribution. The linearity just follows from the definition. The continuity is seen simply by $|\langle \delta, \varphi_m - \varphi \rangle| = |\varphi_m(\mathbf{0}) - \varphi(\mathbf{0})| \leq \sup_{\mathbf{x}} |\varphi_m(\mathbf{x}) - \varphi(\mathbf{x})|$. Then, $\langle \delta, \varphi_m \rangle$ converges to $\langle \delta, \varphi \rangle$ in $\mathbb{C}$ as $m \to \infty$ from the linearity. Moreover, one can show that it is not a regular. For this, for any test function $\varphi \in C_c^\infty(\mathbb{R}^n)$ with $\mathbf{0} \notin \mathrm{supp}(\varphi)$, we would have $0 = \varphi(\mathbf{0}) = \langle \delta, \varphi \rangle = \int_{\mathbb{R}^n} f(\mathbf{x}) \varphi(\mathbf{x}) \, d\mathbf{x}$. This leads to a contradiction since there is no locally integrable function f satisfying the above condition unless it is zero almost everywhere. Despite of this fact, it is customary to write symbolically in physics literature that

$$\varphi(\mathbf{0}) = \langle \delta, \varphi \rangle = \int_{\mathbb{R}^n} \delta(\mathbf{x}) \; \varphi(\mathbf{x}) \; d\mathbf{x} \; . \tag{A.22}$$

This formula simply says that one can formally write a purely symbolic function $\delta(\mathbf{x})$ associated with the Dirac delta distribution. In the beginning formal formulation of our main problem in this thesis, we will use the same notation.

When the test functions are chosen to be Schwartz space $S(\mathbb{R}^n)$, then the distributions defined on them are called as *tempered distributions*. Such distributions are particularly useful when we consider the Fourier transformation of distributions.

One can also define the products of distributions with smooth functions and the derivatives of the distributions. The product of a distribution t with a smooth function ψ is defined by $\langle t\psi, \varphi \rangle = \langle t, \psi\varphi \rangle$ for any $\varphi \in \mathcal{D}(\mathbb{R}^n)$. Smoothness of the function $\psi(\mathbf{x})$ ensures that the product $\psi\varphi$ is in $\mathcal{D}(\mathbb{R}^n)$. In particular, $\langle \psi\delta, \varphi \rangle = \langle \delta, \psi\varphi \rangle = \psi(\mathbf{0})\varphi(\mathbf{0}) = \langle \psi(\mathbf{0})\delta, \varphi \rangle$ for all $\varphi \in \mathcal{D}$, which can be formally written as $\psi(\mathbf{x})\delta(\mathbf{x}) = \psi(\mathbf{0})\delta(\mathbf{x})$.

The distributional derivative of a distribution is defined by $\langle t', \varphi \rangle := -\langle t, \varphi' \rangle$ for any $\varphi \in \mathcal{D}(\mathbb{R}^n)$. The Laplacian of a distribution on $\mathbb{R}^n$ is similarly given by $\langle \Delta t, \varphi \rangle := \langle t, \Delta\varphi \rangle$ for any $\varphi \in \mathcal{D}(\mathbb{R}^n)$. In general, $\langle \partial^k t, \varphi \rangle := (-1)^k \langle t, \partial^k \varphi \rangle$ for any $\varphi \in \mathcal{D}(\mathbb{R}^n)$.

APPENDIX B

FOURIER TRANSFORM OF FUNCTIONS AND DISTRIBUTIONS

This Appendix is written for the purpose of giving the necessary elementary notions of Fourier transformations needed in the thesis without giving the proofs of some theorems. The proofs can be found in (Appel, 2007; Reed and Simon, 1972). Fourier transform can be defined in various spaces. It is natural to define them first on Lebesgue integrable functions $L^1(\mathbb{R}^n)$, given by

$$\mathcal{F}(\varphi(\mathbf{x})) = (\mathcal{F}\varphi)(\mathbf{p}) = \hat{\varphi}(\mathbf{p}) := \int_{\mathbb{R}^n} e^{-i\mathbf{p}\cdot\mathbf{x}} \varphi(\mathbf{x}) \, d\mathbf{x} \; , \tag{B.1}$$

where $\mathbf{p} \cdot \mathbf{x} = \sum_{j=1}^n p_j x_j$. It is customary to use $\mathbf{p}$ or $\mathbf{k}$ as the independent variable for the Fourier transformed functions in physics. One way to see this is to consider the argument of the exponential in the definition of Fourier transformation. The argument of the exponential must be a dimensionless quantity so that the variable in front of $\mathbf{x}$ must be in the dimension of momentum or wave number. For this reason, we simply say that the Fourier transformation map the coordinate space to the momentum space. However, there is no difference from the mathematical point of view and they are both vectors in $\mathbb{R}^n$.

Proposition B.1 *Let $\varphi \in L^1(\mathbb{R}^n)$. Then, $\hat{\varphi}(\mathbf{p})$ is bounded, i.e.,* $\sup |\hat{\varphi}(\mathbf{p})| \leq ||\varphi||_{L^1}$*, and continuous. Moreover,* $\lim_{|\mathbf{p}| \to \infty} |\hat{\varphi}(\mathbf{p})| = 0$.

The proofs of these statements are not difficult. Boundedness is just a simple consequence of the definition. Continuity follows from the fact that $|e^{-i\mathbf{p}\cdot\mathbf{x}} \varphi(\mathbf{x})| = |\varphi(\mathbf{x})| \in L^1(\mathbb{R}^n)$ and Lebesgue dominated convergence theorem ((Rudin, 1976)). The decaying property of $|\hat{\varphi}(\mathbf{p})|$ is coming from the Riemann-Lebesgue lemma. The last statement gives also a clue about the fact that there is a relation between the class of the functions and the decaying properties of its Fourier transform. In particular, one can show that if k th derivative of

$\varphi(x)$ is integrable, then $\hat{\varphi}(p)$ decays at least as fast as $1/p^k$ (it is a simple consequence of the Fourier transform of the derivative of the function and Fourier transform of the function multiplied by x^k, see for the details in (Appel, 2007)).

The problem with the definition of Fourier transform on $L^1(\mathbb{R}^n)$ is that it is not necessary that $\hat{\varphi}(\mathbf{p})$ must also be in $L^1(\mathbb{R}^n)$, that is, Fourier transform does not leave the space stable. This means that the inverse is not always well-defined and one must impose some extra regularity conditions in order to ensure that $\hat{\varphi}(\mathbf{p})$ is in $L^1(\mathbb{R}^n)$ and the existence of its inverse map. For this reason, a more convenient space on which the Fourier transform is defined is the dense subspace of $L^1(\mathbb{R}^n)$ or $L^2(\mathbb{R}^n)$, i.e., rapidly decaying smooth functions, namely Schwartz space $S(\mathbb{R}^n)$. Schwartz space also makes it possible to define the Fourier transform on distributions and some proofs of theorems in multi-dimensional setting is easier (Constantin, 2016; Serov, 2017). For our own convenience, we now state some useful results in Fourier theory without giving the details of the proofs:

Proposition B.2 *If $\varphi \in S(\mathbb{R}^n)$, then $\hat{\varphi} \in S(\mathbb{R}^n)$.*

The idea of the proof is based on the possibility of using the Fourier transform under differentiation and multiplication. Furthermore, we have the following useful result: if $\varphi \in C_c^\infty(\mathbb{R}^n)$, then $\varphi \in S(\mathbb{R}^n)$, see (Appel, 2007; Kanwal, 2012). One can further show that

Theorem B.3 *(Kanwal, 2012) Fourier transformation is a bijective linear continuous map on $S(\mathbb{R})$.*

For $\varphi \in S(\mathbb{R}^n)$, we have Fourier inversion formula

$$\varphi(\mathbf{x}) = \mathcal{F}^{-1}(\hat{\varphi}(\mathbf{p})) = (\mathcal{F}^{-1}\hat{\varphi})(\mathbf{x}) := \int\limits_{\mathbb{R}^n} e^{i\mathbf{p}\cdot\mathbf{x}}\, \hat{\varphi}(\mathbf{p})\, \frac{d\mathbf{p}}{(2\pi)^n}\ , \tag{B.2}$$

and the so-called Plancherel theorem

$$\int\limits_{\mathbb{R}^n} |\varphi(\mathbf{x})|^2\, d\mathbf{x} = \int\limits_{\mathbb{R}^n} |\hat{\varphi}(\mathbf{p})|^2\, \frac{d\mathbf{p}}{(2\pi)^n}\ . \tag{B.3}$$

Moreover, one can show the following important and useful result

$$\mathcal{F}\left(-\Delta\varphi\right)(\mathbf{p}) = |\mathbf{p}|^2\hat{\varphi}(\mathbf{p}) \; . \tag{B.4}$$

Since Schwartz space is dense in $L^2(\mathbb{R}^n)$, and Fourier transform is a linear and continuous map, it can be uniquely extended to an isometric map of $L^2(\mathbb{R}^n)$ onto $L^2(\mathbb{R}^n)$ thanks to the BLT theorem 3.22. One can also extend the definition of Fourier transform for distributions:

Definition B.4 *The Fourier transform of a tempered distribution $t \in \mathcal{S}'(\mathbb{R}^n)$ is defined by*

$$\langle \mathcal{F}(t), \varphi \rangle := \langle t, \mathcal{F}(\varphi) \rangle \; , \tag{B.5}$$

for any $\varphi \in \mathcal{S}(\mathbb{R}^n)$.

Using the above definition, we can find the Fourier transform of Dirac δ distribution as follows:

$$\langle \mathcal{F}\delta, \psi \rangle = \langle \delta, \mathcal{F}\psi \rangle = \langle \delta, \hat{\psi} \rangle := \hat{\psi}(\mathbf{0}) \; . \tag{B.6}$$

From the Fourier transform of $\psi(\mathbf{x})$

$$\hat{\psi}(\mathbf{0}) = \int\limits_{\mathbb{R}^n} e^{-i\mathbf{p}\cdot\mathbf{x}}\psi(\mathbf{x})\; d\mathbf{x}\Big|_{\mathbf{p}=\mathbf{0}} = \int\limits_{\mathbb{R}^n} \psi(\mathbf{x})\; d\mathbf{x} = \langle 1, \psi \rangle \; . \tag{B.7}$$

Hence we get $\langle \mathcal{F}\delta, \psi \rangle = \langle 1, \psi \rangle$, i.e., formally

$$\mathcal{F}\delta = 1 \; . \tag{B.8}$$

Example B.5 *The calculation of $\mathcal{F}(\delta\psi)$:*

$$\langle \mathcal{F}(\delta\psi), \varphi \rangle \;\; = \;\; \langle \mathcal{F}(\delta\psi(\mathbf{0})), \varphi \rangle \; , \tag{B.9}$$

for any test function φ. Since $\mathcal{F}$ is linear and $\psi(\mathbf{0})$ is constant we have

$$\langle \mathcal{F}(\delta\psi(\mathbf{0})), \varphi\rangle = \psi(\mathbf{0})\langle \mathcal{F}\delta, \varphi\rangle = \psi(\mathbf{0})\langle 1, \varphi\rangle = \langle \psi(\mathbf{0}), \varphi\rangle \ . \tag{B.10}$$

Formally, this means Fourier transform of $\delta\psi$ is $\psi(\mathbf{0})$ which can be found by inverse Fourier transform

$$\mathcal{F}(\delta\psi) = \psi(\mathbf{0}) = \int_{\mathbb{R}^n} e^{i\mathbf{p}\cdot\mathbf{x}}\hat{\psi}(\mathbf{p})\ \frac{d\mathbf{p}}{(2\pi)^n}\Bigg|_{\mathbf{x}=\mathbf{0}} = \int_{\mathbb{R}^n} \hat{\psi}(\mathbf{p})\ \frac{d\mathbf{p}}{(2\pi)^n} \ . \tag{B.11}$$

One can also define the so-called Sobolev spaces $H^s(\mathbb{R}^n)$ in terms of distributional derivatives:

$$H^s(\mathbb{R}^n) := \{\varphi \in L^2(\mathbb{R}^n) : \partial^{\mathbf{k}}\varphi \in L^2(\mathbb{R}^n)\ for\ all\ \mathbf{k},\ \text{where } |\mathbf{k}| \leq s\} \ ,$$

where the partial derivatives must be understood in the distributional sense.

Thanks to the Fourier transformation, we have an equivalent characterization of Sobolev spaces (Gustafson and Sigal, 2011), (Hall, 2013): $\varphi \in H^s(\mathbb{R}^n)$ if and only if the following integral

$$\int_{\mathbb{R}^n} (1 + |\mathbf{p}|^2)\hat{\varphi}(\mathbf{p})\ \frac{d\mathbf{p}}{(2\pi)^n} \tag{B.12}$$

is finite. One can also express the Sobolev spaces in terms of absolutely continuous functions (Schmüdgen, 2012).

APPENDIX C

FURTHER ELEMENTARY NOTIONS AND THE PROOFS OF SOME THEOREMS

C.1. The Proof of Bounded Linear Transformation Theorem

We construct a candidate extension for T. Since $D(T)$ is dense in $\mathcal{H}$, for any $\varphi \in \mathcal{H}$ we can find a sequence $\{\varphi_m\}_{m=1}^{\infty}$ in $D(T)$ converging to φ. Since φ_m is convergent, it is Cauchy on $D(T)$. We use linearity and the boundedness of T (the inequality 3.6) to get

$$
\begin{aligned}
||T\varphi_n - T\varphi_m|| &= ||T(\varphi_n - \varphi_m)|| && \text{(C.1)} \\
&\leq ||T||\,||\varphi_n - \varphi_m|| \,, && \text{(C.2)}
\end{aligned}
$$

for every $n, m \in \mathbb{N}$. This means $\{T\varphi_m\}_{m=1}^{\infty}$ is a Cauchy sequence in $\mathcal{H}$ so that it converges to some element of $\mathcal{H}$. From this observation, we will define the following operator (a candidate for the extension):

$$
\begin{aligned}
\hat{T} : \mathcal{H} &\rightarrow \mathcal{H} && \text{(C.3)} \\
\varphi &\mapsto \hat{T}\varphi := \lim_{m \to \infty} T\varphi_m \,, && \text{(C.4)}
\end{aligned}
$$

where $\{\varphi_m\}_{m=1}^{\infty}$ is any sequence in $D(T)$ converging to φ. The problem here could arise since the above definition of $\hat{T}$ may be sequence dependent. Therefore, one must show that the operator $\hat{T}$ is actually well-defined. For this, suppose there are two sequences $\{\varphi_m\}_{m=1}^{\infty}$ and $\{\psi_m\}_{m=1}^{\infty}$ converging to the same vector φ. Then, using the linearity and boundedness and the triangle inequality, we obtain

$$
||T\varphi_m - T\psi_m|| = ||T(\varphi_m - \psi_m)|| \leq ||T||\,||\varphi_m - \varphi + \varphi - \psi_m||
$$

$$\leq \quad ||T||\,(||\varphi_m - \varphi|| + ||\varphi - \psi_m||)\ .$$

Hence, $\hat{T}$ is well-defined. Is $\hat{T}$ an extension of the original operator T that we have started with? To see this, we choose a constant sequence such that all term is φ, i.e., $\{\varphi_m\}_{m=1}^{\infty} := \{\varphi, \varphi, \varphi, \ldots\}$ in $D(T)$. Then

$$\begin{aligned} \hat{T}\varphi &= \lim_{m\to\infty} T\varphi_m \\ &= \lim_{m\to\infty} T\varphi \\ &= T\varphi\ . \end{aligned}$$

Consider a sequence $\{z\varphi_m + \psi_m\}$ in $D(T)$. Then, we have

$$\begin{aligned} \hat{T}(z\varphi + \psi) &= \lim_{m\to\infty} [T(z\varphi_m) + T\psi_m] \\ &= \lim_{m\to\infty} zT\varphi_m + \lim_{m\to\infty} T\psi_m \\ &= z\hat{T}\varphi + \hat{T}\psi\ , \end{aligned}$$

for any $\varphi, \psi \in \mathcal{H}$, $z \in \mathbb{C}$ and φ_n, ψ_m are sequences in $D(T)$ that converges to φ and ψ respectively. This shows that $\hat{T}$ is linear. Using definition of $\hat{T}$ and continuity of norm map, we have

$$\begin{aligned} ||\hat{T}\varphi|| &= ||\lim_{m\to\infty} T\varphi_m|| \\ &= \lim_{m\to\infty} ||T\varphi_m|| \\ &\leq \lim_{m\to\infty} ||T||\,||\varphi_m|| = ||T||\,||\varphi||\ . \end{aligned}$$

Therefore $\hat{T}$ is bounded. As for the uniqueness, suppose there is another extension $\tilde{T}$ of T. Let $\varphi \in \mathcal{H}$ and $\{\varphi_m\}_{m=1}^{\infty}$ be a sequence in $D(T)$ converging to φ. Then, we have

$$||\tilde{T}\varphi - T\varphi_m|| = ||\tilde{T}\varphi - \tilde{T}\varphi_m|| \leq ||\tilde{T}||\,||\varphi - \varphi_m||\ .$$

Then, it follows that $\tilde{T}\varphi = \lim_{n\to\infty} T\varphi_n = \hat{T}\varphi$ for all φ in $\mathcal{H}$. This completes the proof that $\hat{T}$ is the unique bounded linear extension of T. $\square$

C.2. Proof of Closed Graph Theorem

Suppose $\Gamma(T)$ is closed. Therefore $\Gamma(T)$ is a subspace of the Banach space $X \oplus Y$, since T is linear. Since closed subspace of a Banach space is Banach, $\Gamma(T)$ is Banach in the norm

$$||(\varphi, T\varphi)|| = ||\varphi|| + ||T\varphi|| \ . \tag{C.5}$$

Let π_1, π_2 be projection maps such that

$$\begin{aligned} \pi_1 : (\varphi, T\varphi) &\mapsto \varphi \\ \pi_2 : (\varphi, T\varphi) &\mapsto T\varphi \ , \end{aligned}$$

for all $\varphi \in D(T)$. We can show π_i are bijective mappings

$$\begin{aligned} \pi_1(\varphi_1, T\varphi_1) &= \pi_1(\varphi_2, T\varphi_2) \\ \varphi_1 &= \varphi_2 \ . \end{aligned}$$

Then

$$(\varphi_1, T\varphi_1) = (\varphi_2, T\varphi_2) \ , \tag{C.6}$$

which says π_1 is one-to-one. For any $\varphi \in D(T)$ there exists $(\varphi, T\varphi)$ such that

$$\pi_1(\varphi, T\varphi) = \varphi \ . \tag{C.7}$$

So π_1 is onto. Hence it is bijective. Using the same procedure, one can show π_2 is also a bijection.

$$||\pi_1(\varphi, T\varphi)|| = ||\varphi|| \ , \tag{C.8}$$

for any $\varphi \in D(T)$. So it is continuous(bounded). Then its inverse π_1^{-1} is also continuous by inverse mapping theorem. Hence

$$T = \pi_2 \circ \pi_1^{-1} \tag{C.9}$$

is continuous.

Conversely, let $\{(\varphi_m, T\varphi_m)\}_{m=1}^{\infty}$ be a sequence in $\Gamma(T)$ such that $(\varphi_m, T\varphi_m) \to (\varphi, \psi)$. Our aim is to show $(\varphi, \psi) \in \Gamma(T)$, i.e., $\varphi \in D(T)$ and $\psi = T\varphi \in Ran(T)$. But, since T is continuous, we have more than that. $\varphi_m \to \varphi$ implies that $T\varphi_m \to \psi$ and $\psi = T\varphi$. $\square$