BACHELOR

An Introductory Mathematical Overview of the Schrödinger Model of Quantum Mechanics

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1 Introduction

This bachelor thesis aims to introduce quantum mechanics to mathematicians with a basic understanding of functional analysis. Physicists often have their own style and notation, that can be difficult to understand for the average pure mathematician. Yet mathematics is fundamental to quantum mechanics, and much of our understanding of quantum mechanics follows directly from the mathematical models used to describe quantum mechanics. Conversely, quantum mechanics has had a strong influence on the development of some mathematical fields, including spectral theory and the theory of Hilbert spaces. So much so that quantum mechanics sometimes has dedicated chapters in pure functional analysis courses. This makes quantum mechanics a prime example of the real-world application of abstract mathematics. This thesis will outline what quantum mechanics is, why it was developed, and what mathematical concepts and tools are used to build and understand the Schrödinger model of Quantum mechanics.

This thesis will begin by providing a brief historical background to the development of the quantum mechanical model. In the chapter that follows, we will briefly provide some physical insights to inform and justify the assumptions and requirements of the model, before properly defining the necessary mathematical definitions, theorems, and concepts to build the model and describe solutions to the model. In chapter 4 we will use this knowledge to model the free electron, meaning an electron that is not subject to any outside forces. This free electron model will then be compared to how a similar free particle might behave in classical Newtonian mechanics.

2 Physical Background

The birth of quantum mechanics as we know it is commonly attributed to Max Planck's early 20th century work into black body radiation [1]. His research related to understanding how objects, specifically idealized non reflective object, radiate light at different frequencies depending on their temperature. At this point, light was understood to consist of continuous waves with frequencies on a spectrum. The classical model of radiation predicted that black bodies would generate light at all frequencies. The energy released was predicted by the models to be arbitrarily high at high frequencies, a concept called the ultraviolet catastrophe. However, this catastrophe did not show up in experiments, implying a limitation of the model. Planck's work aimed to adjust the traditional model to account for this by introducing a limiting term. His model was successful, but as a result of his model he postulated that the energy of light was released only as multiples of some elemental quantity. To him this was just a theoretical solution, but Einstein then used it to create the concept of photons [2]. He postulated that the energy of light came in localized packets with a proper momentum, despite the wave being spread over larger space. This concept became known as wave-particle duality. The energy of photons interacts with the world as if they are particles, yet they also followed Maxwell's wave theory. This concept turned out to extend to many other small particles, including electrons.

A famous experiment that shows the intriguing behavior of these wave particles is the double slit experiment. This experiment was first performed by Thomas Young in the early 19th century and was the impetus to considering light as waves rather than particles. The experiment has been repeated many times, and in the early 20th century it was used to show that electrons indeed also behave both as waves and particles. At the time it was not yet possible to individually register photons and electrons during the experiment, but with modern technology this can be done.[3] The principle of the experiment is as follows. Some electron source, or light source, is set up across from a screen that can observe the electrons. In between the source and observing screen we place a second screen containing two slits. The electrons can pass this second screen only through the two slits. A classical particle model would predict that the electrons would move from the source, through one of the two slits, onto two spots, or allowing for error, bands, on the observing screen, one for each slit respectively. Furthermore, if we close either slit, we should be able to see that the projection on the screen is the same as the combined contributions of both slits separately. However, this is not what happens. Instead we see an interference pattern emerge. Despite the intensity of both slits independently being high in some spots of the screen, the electrons seem to cancel each other out, allowing the intensity in such a spot with both slits open to still be low. What is even more strange is that when electrons are released and observed individually, the location they hit seems to still follow a distribution with this interference pattern. Apparently, the location of these electrons is dictated directly by some wave-like

property.

Based on this experiment we draw two important conclusions. First is that the behavior of electrons, even individually, is inherently random, and not just a result of experimental error. The second is that the probability distribution of the location of this electron is dictated by some underlying wave-like property.

While this wave-particle duality was a hot topic, Erwin Schrödinger decided to try and create a proper three-dimensional wave equation to try and model the wave mechanics of these particles. This led to what is known as the Schrödinger equation. Although this was not the only attempt at describing this wave-like property, it did lead to the prevailing model of quantum mechanics. This model is what we hope to present in this paper.

3 The Schrödinger Model

3.1 Physical Requirements

In this section we briefly lay out some of the physical assumptions and physical insights that motivate the construction of the Schrödinger model of quantum mechanics. This way we can propose some key requirements and assumptions of the model and its relevant solutions, before we properly define and analyse the system mathematically. As this thesis intends to present the Schrödinger model in a mathematical light, some of these physical assumptions may be taken for granted, without discussing the physical reasoning behind these assumptions in detail.

The mathematics used in this thesis will build primarily on knowledge of functional analysis. The reader is expected to have some of this knowledge handy, but can consult Erwin Kreyszig's book titled Introductory Functional Analysis with Applications [4] for much of this assumed knowledge. The structure of the physics will largely follow the guidelines set out in the early chapters of Gustafson and Sigal's 'Mathematical Concepts of Quantum Mechanics' [5].

In nature many tiny particles, if not all particles, seem to display a random behavior. We call such random particles, like photons or electrons, *quantum particles*. Although there is an inherent randomness to these particles, there does appear to be some underlying deterministic behavior that dictates the probability distributions of these particles. Quantum mechanics attempts to describe this underlying wave-like behavior, thus allowing us to make predictions about the location and behavior of quantum particles as they evolve over time. We model the behaviour of these particles using *wave functions* (or *state vectors*): complex-valued functions $\psi(x)$, where $x \in \mathbb{R}^3$ denotes a location in space. The complex nature of these functions will allow the model to express wave-like properties, like oscillations or the interference pattern between overlapping waves.

Definition 3.1. A mapping ψ is called a *wave function* if it is a square-integrable mapping such that

$$\begin{array}{rccc} \psi: & \mathbb{R}^3 & \to & \mathbb{C}, \\ & x & \mapsto & \psi(x), \end{array} \tag{1}$$

$$\int_{\mathbb{R}^3} |\psi(x)|^2 dx < \infty. \tag{2}$$

The wave function is used to describe and predict the state of our quantum particle. Thus there has to be a way to derive an appropriate probability distribution for the particle's position from this wave function. This probability distribution is given by the function $f = |\psi|^2$:

$$P(\text{a particle is in some region } S \text{ in space}) = \int_S |\psi(x)|^2 dx.$$

We can easily see how an interference pattern could emerge from this model. Say for instance that some particle is governed by a wave state combining two components, $\psi(x) = \psi_1(x) + \psi_2(x)$ where $\psi_1(x) = i$ and $\psi_2(x) = -i$. Then the combined wave function at point x is $\psi(x) = 0$. Then clearly $|\psi(x)|^2 = 0 \neq 2 = |\psi_1(x)|^2 + |\psi_2(x)|^2$. In this case the components of the wave function corresponding to ψ_1 and ψ_2 interfere in x, in fact they cancel each other.

The requirement that $|\psi|^2$ forms a probability distribution for the particle imposes the additional requirement of *normalization*:

$$\int_{\mathbb{R}^3} |\psi(x)|^2 dx = 1. \tag{3}$$

This normalization requirement turns out to be very useful, in that it allows us to restrict ourselves to wave functions that are square-integrable. We use this to justify restricting ourselves to equivalence classes under this *square-integral* norm, as we will discuss in a bit.

Definition 3.2. A function $f : \mathbb{R}^3 \to \mathbb{C}$ is called *square-integrable*, if its *square-integral*, given by

$$\int_{\mathbb{R}^3} |f(x)|^2 dx, \tag{4}$$

exists (and is finite).

The square-integral norm is the squareroot of this square-integral:

$$||\psi|| := \sqrt{\int_{\mathbb{R}^3} |\psi(x)|^2 dx}. \tag{5}$$

The set of all such wave functions is the set

$$\mathcal{L}^2(\mathbb{R}^3) = \{\psi : \mathbb{R}^3 \to \mathbb{C} | \int_{\mathbb{R}^3} |\psi(x)|^2 dx < \infty\}.$$

Sadly, this set $\mathcal{L}^2(\mathbb{R}^3)$ does not form a very convenient space to work in for our purpose, because the square-integral is not a proper norm in this set. For example, one might come up with a pair of wave functions that are equal everywhere except in some finite set of points $\{x_0...x_n\}$. Their difference then is non-zero only on finite points in space, so that its square-integral is 0, which violates one of the key properties of norms. Yet, these functions will be physically indistinguishable. We use this reasoning to justify instead considering the Lebesgue space (or L^p space) $L^2(\mathbb{R}^3)$, where functions that agree almost everywhere are considered equivalent, thus allowing us to use the square root of the square-integral as

its norm. Technically speaking, this means that elements of $L^2(\mathbb{R}^3)$ are equivalence classes, instead of individual functions as we usually see them. Technically speaking, this means that often $\psi(x)$ is not even necessarily well-defined [6, p38]. As a result of this, we aim to express solutions and proofs in the form of Lebesgue integrals. Crucial to these notations is the following lemma.

Lemma 3.1 (Equality)**.** *[4, Lemma 3.8.2] If for some $\phi_1, \phi_2 \in X$ some inner product space $\langle \phi_1, \psi \rangle = \langle \phi_2, \psi \rangle$ for all $\psi \in X$, then $\phi_1 = \phi_2$.*

If we know the state of some quantum particle at some point in time t_0, in the form of a wave function, $\psi_0 \in L^2(\mathbb{R}^3)$, we would like to be able to describe how the state of the particle changes over time. As such, we will usually consider time-dependent wave functions, $\psi(x,t) : \mathbb{R}^3 \times \mathbb{R} \to \mathbb{C}$. These functions effectively form subsets of the function space, where $\psi(\cdot, t)$ is the wave function that denotes the state of a particle at time t,

$$\begin{array}{rccc} \psi(\cdot,t): & \mathbb{R}^3 & \to & \mathbb{C} \\ & x & \mapsto & \psi(x,t). \end{array} \tag{6}$$

Although we assume that there is randomness in the expression of the particles that these wave functions describe, the wave function itself is assumed to be subject to the causality principle: the future states of the system can be fully predicted based on the current state of the system. Similarly, although we have seen in the interference pattern that the contribution of multiple alternatives do not sum properly, we assume that the wave function does follow this principle, called the superposition principle. These assumptions allow us to consider an evolution equation

$$\frac{d}{dt}\psi = A\psi \tag{7}$$

for some linear operator A. Furthermore, the system needs to match our understanding of physics on a larger scale, which informs us of what the operator A should look like. According to classical mechanics, the evolution of a system is described by Newton's laws of motion. In quantum mechanics, we find Schrödinger's equation:

$$i\hbar \frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{2m}\Delta_x \psi(x,t) + V(x)\psi(x,t), \tag{8}$$

where $\hbar$ is the Planck constant, m is the mass of the particle, $\Delta_x = \sum_i \frac{\partial^2}{\partial x_i^2}$ is called the Laplace operator and represents the kinetic energy of the system, and $V(x)$ is a multiplication operator that represents the energy potentials of the system. We call the operator $H = -\frac{\hbar^2}{2m}\Delta_x + V(x)$ the Schrödinger operator of a system, and it is indeed linear.

The behavior of these wave functions comes together in the Cauchy problem, or otherwise

known as the initial value problem,

$$\begin{cases} i\hbar\frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{2m}\Delta_x\psi(x,t) + V(x)\psi(x,t) \\ \psi(x,t_0) = \psi_0(x). \end{cases} \tag{9}$$

The solutions of this Cauchy problem are the objects of interest to us.

3.2 Operator Theory

Now that we have a well-defined mathematical basis of what wave functions are and the spaces they are in, we would like to start gathering the tools necessary to further construct and analyse the dynamics of the model. Does the Cauchy problem (9) have solutions, what would these solutions look like, and in what ways do they match our expectations from the physical reality? Some of these key analytical tools will be presented in this section. We begin by describing the space of compactly supported smooth functions. As we discussed in the previous section, $L^2(\mathbb{R}^3)$ is a set of equivalence classes. Furthermore, as we will see, quite a few of the most important operators will not be well-defined on all of $L^2(\mathbb{R}^3)$. Therefore, we will define a convenient dense subset that we can use to prove most of our theorems, and then extend these to our Hilbert space $L^2(\mathbb{R}^3)$.

Definition 3.3. the linear space, or vector space, of compactly supported smooth functions from R^3 to $\mathbb{C}$ is $C_c^\infty(\mathbb{R}^3)$. Thus, it is the set of all functions ϕ such that,

$$\begin{aligned} &\text{i) } \phi : \mathbb{R}^3 \to \mathbb{C}, \\ &\text{ii) foreach } \phi \text{ there is a } U \subset \mathbb{R}^3 \text{ bounded and closed s.t. } \forall x \in U^c : \phi(x) = 0, \\ &\text{iii) } \tfrac{\partial^k}{\partial x_i{}^k}\psi \text{ exists for any } k \in \mathbb{N}, i \in \{1,2,3\}. \end{aligned} \tag{10}$$

Because these functions are smooth and compactly supported, all such functions are square-integrable. In fact $C_c^\infty(\mathbb{R}^3)$ forms a normed space with the square-integral as its norm. Before we prove this, we take this one step further.

Lemma 3.2. *The linear space of continuously differentiable compact functions $C_c^\infty(\mathbb{R}^3)$ forms an inner product space under the inner product*

$$\begin{array}{rccl} \langle\cdot,\cdot\rangle : & C_c^\infty(\mathbb{R}^3) \times C_c^\infty(\mathbb{R}^3) & \to & \mathbb{C} \\ & \psi, \phi & \mapsto & \int_{\mathbb{R}^3} \psi(x)\overline{\phi(x)}dx, \end{array} \tag{11}$$

where $\overline{a}$ indicates the complex conjugate of $a \in \mathbb{C}$. Henceforth we will use $C_c^\infty(\mathbb{R}^3)$ to indicate both this inner product space and linear space. Similarly we the inner product on $L^2(\mathbb{R}^3)$ is defined as

$$\begin{array}{rccl} \langle\cdot,\cdot\rangle : & L^2(\mathbb{R}^3) \times L^2(\mathbb{R}^3) & \to & \mathbb{C} \\ & \psi, \phi & \mapsto & \int_{\mathbb{R}^3} \psi(x)\overline{\phi(x)}dx. \end{array} \tag{12}$$

The norm induced by this inner product then indeed is the square root of the square-integral,

$$||\psi||^2 = \langle\psi,\psi\rangle = \int_{\mathbb{R}^3} \psi(x)\overline{\psi(x)}dx = \int_{\mathbb{R}^3} |\psi(x)|^2 dx. \tag{13}$$

Although this space $C_c^\infty(\mathbb{R}^3)$ is an inner product space, it is not a Hilbert space, as it is

not closed. One can easily construct a series of functions with infinitely increasing supports. Luckily, inner product spaces can be completed. Recall,

Theorem 3.3. *For any inner product space X, there exists a Hilbert space H and an isomorphism A from X onto a dense subspace $W \subset H$. The space H is unique except for isomorphisms. [4, Thm 3.2.3]*

This completion of $C_c^\infty(\mathbb{R}^3)$ under this inner product forms the Hilbert space that quantum mechanics works in, $L^2(\mathbb{R}^3)$.

Lemma 3.4. *The inner product space $C_c^\infty(\mathbb{R}^3)$ is a dense subspace, and $L^2(\mathbb{R}^3)$ is its completion under the square-integral norm 5.*

The proof to this lemma is far from simple, and is usually proven with the help of the convolution of functions defined later in this chapter. A detailed proof can be found in G. Folland's 'A Guide to Advanced Real Analysis' [7, Prop 6.4]. Generally speaking, the proof approximates functions in $L^2(\mathbb{R}^3)$ by a sequence of smooth functions that are generated using standard smooth functions called *mollifiers*. Sequences of such mollifiers approximate 0 functions with singular discontinuities. An example of such a mollifier is the function

$$\psi(x) = \begin{cases} e^{\frac{1}{|x|^2-1}} \text{ if } |x| < 1 \\ 0 \text{ otherwise.} \end{cases}$$

Recall *The Cauchy problem* 9

$$\begin{cases} i\hbar\frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{2m}\Delta_x\psi(x,t) + V(x)\psi(x,t) = H\psi(x,t) \\ \psi(x,t_0) = \psi_0(x). \end{cases}$$

We call H the *Schrödinger operator* of a given system, and is assumed to be a linear operator $H : \mathcal{D}(H) \subset L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3)$.

As it turns out, the proper existence of solutions to the Cauchy problem is dependent on a concept called self-adjointness. Roughly speaking, self-adjointness combines symmetry, with some features that usually come with boundedness. In section 3.3 self-adjointness will be shown to be needed to conserve the trait that $|\psi(t,\cdot)|^2$ behaves as a probability distribution at all points in time, as well as being necessary to define the exponential of a linear operator, which we will do at the end of this section.

Self-adjointness may be familiar to the reader for bounded operators. There it is a fairly simple concept.

Definition 3.4. A bounded linear operator $T : \mathcal{H} \to \mathcal{H}$ on some Hilbert space $\mathcal{H}$, with inner product $\langle \cdot, \cdot \rangle$, is *self-adjoint*, if the operator is equal to its Hilbert-adjoint operator, $T = T^*$. Where the Hilbert-adjoint operator T^* is defined, s.t. $\langle Tx, y \rangle = \langle x, T^* y \rangle$ for all $x, y \in \mathcal{H}$.

For bounded linear operators, self-adjointness is equivalent to the operator T being symmetric and defined on, and to the whole Hilbert space $\mathcal{H}$.[4, Thm. 3.10.1]

Alternatively, we can use the following theorem to show that symmetric operators defined on dense subsets of some Hilbert space $\mathcal{H}$ can be extended to construct self-adjoint operators.

Theorem 3.5 (Bounded linear extensions.)**.** *Let $T : \mathcal{D}(T) \subset X \to Y$ be a bounded linear operator, where Y is Banach. Then T has an extension $\overline{T} : \overline{\mathcal{D}(T)} \to Y$, so that its closure $\overline{T}$ is defined on all of X, $D(\overline{T}) = X$. [4, Thm. 2.7.11]*

Where closed refers to the following,

Definition 3.5. A linear operator $T : \mathcal{D}(T) \subset \mathcal{H} \to \mathcal{H}$, where $\mathcal{H}$ is a complex Hilbert space, then T is *closed* if and only if

$$x_n \to x \text{ and } Tx_n \to y \text{ in } \mathcal{H} \tag{14}$$

implies that $Tx = y$. [4, Def. 10.3.2]

Sadly, the constraint of considering bounded operators is too strong of a limitation. In quantum mechanics, the Laplacian operator Δ_x for example plays a major role in our model, yet is clearly not bounded. Although it is densely defined on $C_c^\infty(\mathbb{R}^3) \subset L^2(\mathbb{R}^3)$, we quickly run into domain issues when trying to apply the ideas of bounded self-adjointness to this unbounded operator, as it is explicitly undefined on many elements of $L^2(\mathbb{R}^3)$. The following theorem shows how central such domain issues can be for unbounded operators.

Theorem 3.6 (Hellinger-Toeplitz)**.** *If a linear operator T is defined on all of a complex Hilbert Space $\mathcal{H}$, and is Symmetrical, then T is bounded. [4, Thm. 10.1.1]*

Conversely, unbounded symmetrical operators can only be defined on a subset of a complex Hilbert Space, and not the whole Hilbert space.

Theorem 3.7 (Closure of a symmetric operator)**.** *Let $T : \mathcal{D}(T) \subset X \to \mathcal{H}$ be a linear symmetric operator, and $\mathcal{D}(T)$ is dense in X, then it has a unique closure. [4, Thm. 10.3.5]*

We will need to find a way to extend the definition of self-adjointness to unbounded operators, while maintaining some of the relevant features, like symmetry and how it relates to elements to the rest of the Hilbert space.

Definition 3.6. A Linear operator $A : \mathcal{D}(A) \subset \mathcal{H} \to \mathcal{H}$, for some Hilbert space $\mathcal{H}$ is called *Self-Adjoint* if it is symmetric, densely defined on $\mathcal{H}$ and $\mathcal{R}(A + z) = \mathcal{H}$ for all $z \in \mathbb{C} \setminus \mathbb{R}$.

Notice that for bounded self-adjoint operators, by the definition of the adjoint operator, $\mathcal{R}(A) = \mathcal{H}$. So it is easy to see how this definition overlaps with the previous one in the case of bounded operators.

The property that $\mathcal{R}(A + z) = \mathcal{H}$ for complex z might seem like somewhat of an unintuitive distinction to make, and in fact self-adjointness in mathematics is generally defined through the Hilbert-adjoint operator instead (eg. [4, def. 10.2.5]). However, our definition more directly satisfies our needs in this thesis, as it will allow us to define the exponential of an operator at the end of this chapter. To get to a definition of the exponent of operators, we begin by defining the Resolvent operator, which can be used to define sequences of bounded operators that converge to some unbounded operator A.

Definition 3.7. Given a self-adjoint operator A, we define the Resolvent operator R_λ, for $\lambda \in \mathbb{R}$, $\lambda \neq 0$ by

$$R_\lambda(A) := (A - \lambda I)^{-1} \tag{15}$$

Proof. To prove that the resolvent operator is well-defined for all self-adjoint operators, we use the theorem that linear operators are invertible if and only if their null space is $\{0\}$, or $(A + i\lambda)\psi = 0 \iff \psi = 0$. [4, Thm. 2.6.10]

Let some $\phi \in \mathcal{D}(A)$, and some $z \in \mathbb{C}$, $\mu, \lambda \in \mathbb{R}$ so that $z = \lambda + i\mu$ where $\mu \neq 0$. We would like to show that $||(A + z)\phi|| > 0$ for $\phi \neq 0$. Consider $\|(A + z)\phi\|^2 = \langle (A + z)\phi, (A + z)\phi \rangle$ $= \langle (A + \lambda + i\mu)\phi, (A + \lambda + i\mu)\phi \rangle$. Because $(A + \lambda)$ is symmetrical, and $\overline{(i\mu)} = -i\mu$, we can rewrite this as

$$\begin{aligned}
\langle (A + \lambda + i\mu)\phi, (A + \lambda + i\mu)\phi \rangle &= \langle (A + \lambda + i\mu)(A + \lambda - i\mu)\phi, \phi \rangle \\
&= \langle (A + \lambda)(A + \lambda)\phi, \phi \rangle + \langle (A + \lambda)(i\mu)\phi, \phi \rangle \\
&\quad - \langle (A + \lambda)(i\mu)\phi, \phi \rangle + \langle (i\mu)(-i\mu)\phi, \phi \rangle \\
&= ||(A + \lambda)\phi||^2 + ||\mu\phi||^2 \\
&\geq ||\mu\phi||^2.
\end{aligned}$$

So: $\|(A + z)\phi\|^2 \geq ||\mu\phi||^2$, and thus, since μ was assumed to be non zero, if $\phi \neq 0$, $(A+z)\phi \neq 0$. Using the inverse operator theorem mentioned above, this proves that $(A+z)$ is invertible. If we consider $z = -\lambda i$, the Resolvent operator $R_\lambda(A)$ exists. □

Furthermore, since the Resolvent operator is defined on all of $\mathcal{H}$ for self-adjoint operators, by the Hellinger-Toeplitz theorem 3.6, it is bounded. From the proof of the existence of the

resolvent operator, we can also deduce an upper bound estimate, by plugging $\psi = (A+z)\psi$, for $z = i\lambda$ in the final inequality. Although this proof is not sufficient to show that this upper bound is also the norm, we can still use it as an estimate.

$$||R_\lambda(A)\phi|| \leq \frac{1}{|\lambda|}||\phi|| \text{ for } \lambda \neq 0 \tag{16}$$

Resolvent operators are very important in spectral theory. For us, the fact that they are bounded linear operators with a domain on all of $\mathcal{H}$ will be of great use to help us define the exponential of operators.

Lemma 3.8. *For any unbounded self-adjoint operator A, the family of operators defines bounded operators*

$$A_\lambda := \frac{1}{2}\lambda^2\left((A+i\lambda)^{-1} + (A-i\lambda)^{-1}\right) \text{ for } \lambda > 0, \tag{17}$$

such that

$$A_\lambda \to A \text{ as } \lambda \to \infty.$$

A proof for this lemma can be found in the mathematical supplement 6.2.

Definition 3.8. Let A a bounded self-adjoint operator. we define the exponential operator of A as

$$e^{iA_\lambda} := \sum_{n=0}^{\infty} \frac{1}{n!}(iA_\lambda)^n. \tag{18}$$

Definition 3.9. Let A an unbounded self-adjoint operator. we define the exponential operator of A as

$$e^{iA}\psi := \lim_{\lambda\to\infty} e^{iA_\lambda}\psi, \tag{19}$$

where $e^{iA_\lambda}\psi$ is defined according to the definition for bounded operators.

We will prove that the limit statement 19 converges in the Mathematical Supplement, lemma 6.3.

Using the upper bound of 16, we can show that the exponential in both the bounded case 18, and by extension in the unbounded case 19 are both bounded. thus allowing us to extend its definition to all of $L^2(\mathbb{R}^3)$, using the bounded linear extension theorem 3.5.

3.3 Solutions in the Schrödinger Model

Now that we have outlined some important tools in section 3.2, we will use them to analyze the solutions of our Cauchy problem 9, and check these solutions on the physical requirements outlined in 3.1. As stated in the previous section, Self-Adjointness will be a key factor in finding solutions that meet those requirements.

Again, recall the Cauchy Problem,

$$\begin{cases} i\hbar\frac{\partial}{\partial t}\psi(x,t) = -\frac{\hbar^2}{2m}\Delta_x\psi(x,t) + V(x)\psi(x,t) = H\psi(x,t) \\ \psi(x,t_0) = \psi_0(x). \end{cases}$$

We begin by considering the concept of *Conservation of probability*. Given that a given solution $|\psi(x,t)|^2$ needs to function as a probability distribution at any point in time t, we should analyse for our Cauchy problem if or under what conditions the square-integral of the solution remains 1. So, given $||\psi_0|| = 1$, we must have that $||\psi(x,t)||$ is constant over time.

Theorem 3.9. *A solution $\psi(x,t)$ to the Cauchy problem 9 conserves probability if*

$$\frac{d}{dt}||\psi(x,t)|| = \frac{d}{dt}\int_{\mathbb{R}^3}|\psi(x,t)|^2dx = 0. \tag{20}$$

This is true, iff the Schrödinger operator H is symmetric.

Proof. Using the chain rule, $\frac{d}{dt}(\psi(x,t)\overline{\psi(x,t)}) = \overline{\psi(x,t)}\frac{d}{dt}\psi(x,t) + \psi(x,t)\frac{d}{dt}\overline{\psi(x,t)}$, we can rewrite our earlier equality (16),

$$\frac{d}{dt}\langle\psi,\psi\rangle = \langle\dot{\psi},\psi\rangle + \langle\psi,\dot{\psi}\rangle = \langle\frac{1}{ih}H\psi,\psi\rangle + \langle\psi,\frac{1}{ih}H\psi\rangle = \frac{1}{ih}(\langle H\psi,\psi\rangle - \langle\psi,H\psi\rangle) = 0.$$

The final equality here is implies that indeed

$$\frac{d}{dt}||\psi(x,t)|| = 0 \iff \langle H\psi,\psi\rangle = \langle\psi,H\psi\rangle$$

Thus H being symmetric is sufficient to conserve probability. □

Symmetry is not only sufficient, but necessary. This is because $\langle H\psi,\psi\rangle = \langle\psi,H\psi\rangle$ for all $\psi \in \mathcal{H}$ is sufficient to show symmetry. This can be proven using what is known as the Polarization identity. Although the finding is very useful, the proof is very detailed and not particularly interesting, so we refer to [6, Lemma 2.1] for a proof of this statement.

Conservation of probability allows us to prove that for Self-Adjoint operators H, the solution to the Cauchy-problem both conserves probability, and is a unique solution. This

is referred to as *Existence of Dynamics*. Self-Adjointness of the Schrödinger operator is a necessary and sufficient condition for the Existence of Dynamics.

Proof. To prove the uniqueness of solutions, consider $\psi_1(x,t)$, $\psi_2(x,t)$ both solutions to the Cauchy problem with H self-adjoint. Then, $\psi_1(x,0) - \psi_2(x,0) = \psi_0 - \psi_0 = 0$. Using linearity of H, $i\hbar\frac{d}{dt}(\psi_1 - \psi_2)(t) = H(\psi_1 - \psi_2)(t)$, so that $\psi_1 - \psi_2$ is a solution to the Schrödinger equation, and thus conserves probability. Then indeed $||\psi_1 - \psi_2||(t) = 0$ for all t. So the solutions are the equivalent. □

Having now established that the Cauchy problem, given the Schrödinger operator is self-adjoint, has a unique solution that conserves probability, we would like to show that we can use the exponential of an operator to define this unique solution. This solution is given by

$$\psi(x,t) = U(t)\psi_0(x) = e^{-\frac{it}{\hbar}H}\psi_0(x). \tag{21}$$

Theorem 3.10. *For self adjoint operators H, the operator $U(t) = e^{-itH/\hbar}$ according to our definition 3.9 forms a unique family of solutions of bounded operators that define the solutions to the cauchy problem. These operators have the following properties,*

$$i\hbar\frac{\partial}{\partial t}U(t)\psi = HU(t)\psi = U(t)H\psi \text{ on the domain } \mathcal{D}(\frac{\partial}{\partial t}U(t)) = \mathcal{D}(H), \tag{22}$$

$$U(0) = I \tag{23}$$

$$U(t)U(s) = U(t+s), \tag{24}$$

$$||U(t)\psi|| = ||\psi||, \text{ and} \tag{25}$$

$$U(t)\psi \to \psi \text{ as } t \to 0. \tag{26}$$

The properties 22 and 23 combine to show that this indeed forms the evolution operator of our Cauchy problem.

Operators that have properties 23 - 25 are commonly referred to as 'one-parameter unitary operators' in spectral theory, and 26 is referred to as strong continuity of an operator. [8, Def 10.11]

The remainder of this section is dedicated to proving the above theorem. Although it is quite long and might hurt the reading experience, the use of equality lemma 3.1 is well demonstrated in this section. We begin by providing a proof that these properties are true for bounded self-adjoint operators A.

Proof. Consider A, a bounded self adjoint operator on $\mathcal{D}(A) = L^2(\mathbb{R}^3)$, and the exponential

$$U(t) := e^{-itA/\hbar} = \sum_n^\infty \frac{1}{n!}(-\frac{i}{\hbar}tA)^n. \tag{27}$$

i $U(t)$ satisfies equation 8. Consider some $\psi \in D(A) = L^2(\mathbb{R}^3)$. By definition,

$$i\hbar \frac{d}{dt} U(t)\psi = i\hbar \frac{d}{dt} \sum_{n=0}^{\infty} \frac{1}{n!} (-\frac{i}{\hbar} tA)^n \psi.$$

To bring the differential operator into the sum, we point out that the convergence of

$$i\hbar \sum \frac{\partial}{\partial t} \frac{1}{n!} (-\frac{i}{\hbar} tA)^n \psi = A \sum \frac{1}{n!} (-\frac{i}{\hbar} tA)^n \psi$$

is uniform on any interval $t \in [a, b]$, since

$$||A \sum \frac{1}{n!} (-itA)^n \psi|| \leq ||A|| \sum \frac{1}{n!} |t|^n ||A||^n = ||A|| e^{|t|||A||} \leq ||A|| e^{M||A||} < \infty$$

for M the maximum of $|t|$ on some interval $[a, b]$. This allows for the use of the uniform convergence theorem [9, Thm 8.3.5], so that indeed

$$i\hbar \frac{d}{dt} U(t)\psi = i\hbar \frac{d}{dt} \sum_{n=0}^{\infty} \frac{1}{n!} (-\frac{i}{\hbar} tA)^n \psi = i\hbar \sum_{n=0}^{\infty} \frac{d}{dt} \frac{1}{n!} (-\frac{i}{\hbar} tA)^n \psi$$

.

Furthermore, since $A^n\psi$ is constant with respect to t, we can differentiate the terms as follows,

$$\begin{aligned} i\hbar \sum_{n=0}^{\infty} \frac{d}{dt} \frac{1}{n!} (-\frac{i}{\hbar} tA)^n \psi &= i\hbar \sum_{n=0}^{\infty} \frac{n}{n!} t^{n-1} (-\frac{i}{\hbar} A)^n \psi = A \sum_{n=0}^{\infty} \frac{1}{n!} (-\frac{i}{\hbar} tA)^n \psi \\ &= \sum_{n=0}^{\infty} \frac{1}{n!} (-\frac{i}{\hbar} tA)^n \psi A. \end{aligned}$$

Which proves the equality 22.

ii $U(0) = I$ follows directly from the definition of $U(t)$.

iii the proof that $U(t)U(s) = U(t+s)$ follows a very similar line of reasoning to the proof for the similar statement for the traditional exponential function on $\mathbb{R}$. First we use the binomial distribution to split $(t+s)^n$ into multiple terms, then we use the Cauchy product to split the sums, so that

$$\begin{aligned} U(t+s) &= \sum_{n}^{\infty} \frac{1}{n!} \left(-\frac{i}{\hbar} (t+s) A \right)^n = \sum_{n}^{\infty} \frac{1}{n!} \left(\sum_{k}^{\infty} \binom{n}{k} t^k s^{n-k} \right) (-\frac{i}{\hbar} A)^n \\ &= \sum_{n}^{\infty} \frac{1}{n!} t^n (-\frac{i}{\hbar} A)^n \sum_{m}^{\infty} \frac{1}{n!} s^m (-\frac{i}{\hbar} A)^m = U(t)U(s). \end{aligned}$$

iv $||U(t)\psi|| = ||\psi||$. Since $U(0) = I$, and $U(t)\psi$ is a solution to the equation 22 with self adjoint A, we can use the proof of theorem 3.9 to show that $||U(t)\psi||$ is constant over time, thus $U(t)$ is unitary for all t.

v $U(t)\psi \to \psi$ as $t \to 0$. Since we have proven equation 22, and 23, the fundamental theorem of calculus can be applied, so that

$$U(t)\psi - \psi = U(t)\psi - U(0)\psi = \int_0^t \frac{d}{dt}U(s)\psi ds = \int_0^t \frac{1}{i\hbar}U(s)A\psi ds. \tag{28}$$

which indeed converges to 0 as $t \to 0$.

□

Now that we have proven theorem 3.10, for bounded self-adjoint operators A, we will proof that the theorem also holds for unbounded self-adjoint operators.

Proof. Consider an unbounded self-adjoint operator H on $\mathcal{D}(H)$. Define for $t \in \mathbb{R}$

$$U(t) := e^{-\frac{it}{\hbar}H} = \lim_{\lambda\to\infty} e^{-\frac{it}{\hbar}H_\lambda} \tag{29}$$

where H_λ is defined according to equation 17.

i We will prove that 8 holds for $U(t)$, H, by using the equivalence relation under the inner product of $L^2(\mathbb{R}^3)$ explicitly, as discussed in lemma 3.1, to deal with limit issues. Notice also that the statement for operators implies that it works specifically for their respective domains, and so $\mathcal{D}(\frac{\partial}{\partial t}U(t)) = \mathcal{D}(U(t)A)$. Thus we will show that for any $\phi \in \mathcal{D}(H)$: $\langle\phi, i\hbar\frac{\partial}{\partial t}U(t)\psi\rangle = \langle\phi, HU(t)\psi\rangle$. This domain restriction of ϕ is justified by the fact that H is self-adjoint.

Consider

$$i\hbar\frac{\partial}{\partial t}\langle\phi, U(t)\psi\rangle = i\hbar\frac{\partial}{\partial t}\langle\phi, \lim_{\lambda\to\infty} e^{-itH_\lambda/\hbar}\psi\rangle, \tag{30}$$

We can bring the limit statement out of the integral using the dominated convergence theorem, and, as we have seen in the bounded case, $\frac{\partial}{\partial t}e^{-itH_\lambda/\hbar}$ converges uniformly, so we can again use the uniform convergence theorem to exchange the limits, so that

$$i\hbar\frac{\partial}{\partial t}\langle\phi, U(t)\psi\rangle = i\hbar\frac{\partial}{\partial t}\lim_{\lambda\to\infty}\langle\phi, e^{-itH_\lambda/\hbar}\psi\rangle = i\hbar\lim_{\lambda\to\infty}\langle\phi, \frac{\partial}{\partial t}e^{-itH_\lambda/\hbar}\psi\rangle = i\hbar\lim_{\lambda\to\infty}\langle\phi, \frac{\partial}{\partial t}e^{-itH_\lambda/\hbar}\psi\rangle, \tag{31}$$

and again, using the proof that 8 holds for bounded self -adjoint operators, we find that

$$i\hbar\frac{\partial}{\partial t}\langle\phi, U(t)\psi\rangle = \lim_{\lambda\to\infty}\langle\phi, H_\lambda e^{-itH_\lambda/\hbar}\psi\rangle. \tag{32}$$

To finish this proof, we first note that $H_\lambda e^{-itH_\lambda/\hbar}\psi = e^{-itH_\lambda/\hbar}H_\lambda\psi$ and thus, for $\psi \in \mathcal{D}(H)$,

$$\lim_{\lambda\to}\langle\phi, H_\lambda e^{-itH_\lambda/\hbar}\psi\rangle = \lim_{\lambda\to\infty}\langle\phi, e^{-itH_\lambda/\hbar}H_\lambda\psi\rangle, \tag{33}$$

and we can bring the limit into the integral using dominated convergence theorem, so that indeed

$$i\hbar\frac{\partial}{\partial t}\langle\phi, U(t)\psi\rangle = \langle\phi, HU(t)\psi\rangle = \langle\psi, U(t)H\psi\rangle. \tag{34}$$

Furthermore, to recognise that this is also the full domain of $\frac{\partial}{\partial t}U(t)$, we note that otherwise $\lim_{\lambda\to\infty} H_\lambda$ was a proper symmetric extension of H, which violates the self-adjointness of H.

So indeed the equation 8 holds.

ii $U(0) = I$, equation 23 is clearly true, since for $t = 0$

$$\lim_{\lambda\to\infty} e^{-i0H_\lambda} = \lim_{\lambda\to\infty} I = I. \tag{35}$$

iii We will again proof equation 24 using equality. Consider some $\psi, \phi \in L^2(\mathbb{R}^3)$. Using dominated convergence, we can show that

$$\langle\phi, U(t+s)\psi\rangle = \lim_{\lambda\to\infty}\langle\phi, e^{-i(t+s)H_\lambda/\hbar}\psi\rangle. \tag{36}$$

As we have seen that equation 24 in the bounded case, we can split this exponent, so that

$$\langle\phi, U(t+s)\psi\rangle = \lim_{\lambda\to\infty}\langle\phi, e^{-itH_\lambda/\hbar}e^{-isH_\lambda/\hbar}\psi\rangle = \lim_{\lambda\to\infty}\langle e^{itH_\lambda/\hbar}\phi, e^{-isH_\lambda/\hbar}\psi\rangle = . \tag{37}$$

Now, since $e^{itH_\lambda/\hbar}\phi\overline{e^{-isH_\lambda/\hbar}\psi}$ is simply a multiplication of sequences that are known to converge, we can again use the dominated convergence theorem to bring the limit into the integral, so that

$$\langle\phi, U(t+s)\psi\rangle = \langle U(-t)\phi, U(s)\psi\rangle. \tag{38}$$

To complete the proof, we point out that by writing $U(-t)$ as its limit statement, and bringing this to the other side of the inner product, shows that indeed $U(-t) = U(t)^*$, so that we find

$$\langle\phi, U(t+s)\psi\rangle = \langle\phi, U(t)U(s)\psi\rangle, \tag{39}$$

completing the proof by equality 3.1.

iv Following the previous proof of equation 24 we can use that $U(t)^* = U(-t)$, as well

as the fact that $U(-t)U(t) = U(0) = I$ to show proof that indeed

$$||U(t)\psi|| = \langle U(t)\psi, U(t)\psi\rangle = \langle \psi, U(-t)U(t)\psi\rangle = \langle \psi, \psi\rangle = ||\psi||, \tag{40}$$

proving the property of 25

v $U(t)\psi \to \psi$ as $t \to 0$ (strongly continuous). We will proof this for $\psi \in \mathcal{D}(H)$, then by the fact that $D(H)$ is dense in $L2(\mathbb{R}^3)$, and that $U(t)$ is bounded, this property extends to $L^2(\mathbb{R}^3)$.

Consider some $\phi, \psi \in \mathcal{D}(H)$ the function $f(t) = \langle \phi, U(t)\psi\rangle$. As we have seen in the proof of property 8, $f(t)'$ exists on $\mathcal{D}(H)$. By the fundamental theorem of calculus, we know that

$$f(t) - f(0) = \int_0^t f(s)'ds, \tag{41}$$

which goes to 0 as $t \to 0$. Thus indeed $\langle \phi, U(t)\psi\rangle \to \langle \phi, \psi\rangle$. This proofs that $U(t)\psi \to \psi$ as $t \to 0$ in $L^2(\mathbb{R}^3)$.

□

3.4 Fourier Transforms

We now know and have properly defined solutions to the Cauchy problem. However, doing calculations with the operators in equation 21 is far from straightforward, forcing us to deal with complex limit statements. To get the solutions as an expression of the initial value ψ_0, we turn to Fourier transforms. The Fourier Transform is an invertible operator on $L^2(\mathbb{R}^3)$, that has very convenient mappings of differential operators like the Laplacian operator Δ, allowing us to redefine our solutions in the form of integral operators. This makes it a very important operator in the field of Quantum Mechanics.

Definition 3.10. Integral operators are linear operators K such that for some *kernel* function $k(x, y) : \mathbb{R}^3 \times \mathbb{R}^3 \to \mathbb{C}$

$$K\psi(x) = \langle \psi, k(x, .)\rangle = \int_{\mathbb{R}^3} k(x, y)\psi(y)dy. \tag{42}$$

Given $k(x, y) \in L^2(\mathbb{R}^3 \times \mathbb{R}^3)$, the integral operator K is a bounded operator on $L^2(\mathbb{R}^3)$.

Definition 3.11. The Fourier transform of a wave function $\psi \in L^1(\mathbb{R}^3) \cap L^2(\mathbb{R}^3)$ is given by

$$F\psi(x) = (2\pi\hbar)^{-3/2} \int_{\mathbb{R}^3} \psi(y)e^{-\frac{i}{\hbar}y\cdot x}dy, \tag{43}$$

where '$\cdot$' is the dot product on $\mathbb{R}^3$.

The existence and boundedness of the Fourier Transform on $L^1(\mathbb{R}^3)$ is quite straightforward. On $L^2(\mathbb{R}^3)$ however it is harder to prove, but here too it is bounded. This can be proven in multiple ways, most directly by what is known as the *Plancherel Theorem.* [8, A.18]

Since $C_c^\infty(\mathbb{R}^3)$ is dense in $L^2(\mathbb{R}^3)$, as well as consisting of functions that are integrable, we can use the bounded linear extension theorem 3.5 to define $\overline{F} : L^2(\mathbb{R}^3) \to L^2(\mathbb{R}^3)$. The adjoint operator F^* is then its inverse, given by

$$F^{-1}\psi(x) = (2\pi\hbar)^{-3/2} \int_{\mathbb{R}^3} \psi(y)e^{\frac{i}{\hbar}y\cdot x}dy. \tag{44}$$

The usefulness of the Fourier transform lies in how it maps the differential operators, and how it allows us to define integral operators on $L^2(\mathbb{R}^3)$.

Consider the operator $p = -i\hbar\nabla_x$, and some function $\psi \in \mathcal{D}(\Delta)$. We can use the proof that Δ_x is symmetrical (6.1) on its domain $\mathcal{D}(\Delta) \subset L^2(\mathbb{R}^3)$, so that

$$\begin{aligned} F(p\psi)(x) &= (2\pi\hbar)^{-3/2} \int_{\mathbb{R}^3} (-i\hbar\nabla_y)\psi(y)e^{-\frac{i}{\hbar}x\cdot y}dy = (2\pi\hbar)^{-3/2} \int_{\mathbb{R}^3} \psi(y)(-i\hbar\nabla_y)e^{-\frac{i}{\hbar}x\cdot y}dy \\ &= xF\psi(x). \end{aligned}$$

And similarly, consider $|p|^2\psi = -\hbar^2\Delta_x\psi$, where $|.|$ is the vector norm $|k|^2 = \sum_n k_n^2$, where $n = 3$,

$$\begin{aligned} F(|p|^2\psi)(x) &= (2\pi\hbar)^{-3/2}\int_{\mathbb{R}^3}(-\hbar^2\Delta_y)\psi(y)e^{-\frac{i}{\hbar}x\cdot y}dy \\ &= (2\pi\hbar)^{-3/2}\int_{\mathbb{R}^3}\psi(y)(-\hbar^2\Delta_y)e^{-\frac{i}{\hbar}x\cdot y}dy \\ &= |x|^2F\psi(x). \end{aligned} \tag{45}$$

We can use this to easily construct operators as sums of p or $|p|^2$, as long as the sum $\sum_n k_n$ converges in $\mathbb{R}^3$ or $\mathbb{R}$ respectively.

Consider $g(k)$, a function such that $g(k) := \sum_n^\infty a_n|k|^{2n}$, $n \in \mathbb{N}$. Then we can define the operator $g(p)$ on $L^1(\mathbb{R}^3) \cap L^2(\mathbb{R}^3)$ by

$$F(g(p)\psi)(k) = \sum_n^\infty a_n|k|^{2n}F(\psi)(k) = g(k)F\psi(k), \tag{46}$$

and taking the inverse Fourier transform to find $g(p)\psi$.

Definition 3.12. Given a function $g(k)$ on $\mathbb{R}^3$ such that $g(k) = \sum_n^\infty a_n|k|^{2n}$, $n \in \mathbb{N}$, then the operator $g(p)$ on $L^1(\mathbb{R}^3) \cap L^2(\mathbb{R}^3)$ is defined by

$$g(p)\psi(x) := F^{-1}(gF\psi)(x). \tag{47}$$

To get an expression for such an operator in integral operator form, we now define the convolution of functions.

Definition 3.13. Consider functions f, $g \in L^2(\mathbb{R}^3)$, then the *convolution* of f and g is given by

$$(f * g)(x) := \int_{\mathbb{R}^3} f(y)g(y-x)dy. \tag{48}$$

The convolution of function under the Fourier transform has a few useful properties. Most notably are the following:

$$F(f * g) = (2\pi\hbar)^{3/2}F(f)F(g), \text{ and,} \tag{49}$$

$$F(fg) = (2\pi\hbar)^{-3/2}F(f) * F(g). \tag{50}$$

We can use these properties to rewrite the operator $g(p)$ above as an integral operator,

$$F^{-1}F(g(p)\psi)(x) = F^{-1}[g(k)F\psi(k)](x) = (2\pi\hbar)^{-3/2}(F^{-1}g * \psi)(x), \tag{51}$$

which defines a direct expression for the operator as a function of ψ.

4 Free Electron

We will sketch an idea of how quantum mechanics differs from the way we view problems compared to the approach of Classical Mechanics. This difference will be outlined by analyzing the respective models of a free electron, an electron that is not subject to any outside forces or potentials.

4.1 Classical Particle

In classical mechanics we can usually simplify particles as consisting of a constant mass, m, usually centered around a single coordinate in space, the 'center of mass'. We consider this coordinate, denotated by x, to represent the position of our particle in space. We can track this position in space as a function over time:

$$\begin{aligned} x\colon \mathbb{R} &\longrightarrow \mathbb{R}^3 \\ t &\longmapsto x(t) \end{aligned}$$

Considering the location as a function of time allows us to consider the motion of the electron in our model. The velocity of this particle is then given by

$v(t) = \dot{x}(t)$, or, $v(t) = \frac{d}{dt}x(t)$, and its acceleration by $a(t) = \ddot{x}(t)$ or $a(t) = \frac{d^2}{dt^2}x(t)$.

Classical mechanics has models for the acceleration and velocity of this particle that we can use here. Newton's laws, the laws of motion, and the law of inertia show us that, in the problem of our free electron, where there is no outside force applied to our electron, the acceleration of the electron is 0. Using Newton's second law of motion, where the force applied is assumed to be 0, the mass is assumed to be constant, we find for $t \in \mathbb{R}$

$$F = \frac{d}{dt}mv(t) = ma(t) \Longrightarrow ma(t) = 0 \tag{52}$$

We can use this acceleration of 0 to give a better description of the velocity and the position of our electron over time. We call this the *evolution* of our function x. For example, giving a starting position $x_0 \in \mathbb{R}^3$ at time $t_0 \in \mathbb{R}$, we could describe the position of our electron at time $t \in \mathbb{R}$ by

$$\begin{cases} \dot{x}(t) = \int_{t_0}^{t} 0 ds \\ x(t) = \int_{t_0}^{t} \dot{x}(t_0) ds \end{cases} \Longrightarrow \begin{cases} \dot{x}(t) = \dot{x}(t_0) \\ x(t) = \dot{x}(t_0)t + x_0 \end{cases}, \tag{53}$$

or, given some initial velocity $v_0 = \dot{x}(t_0)$:

$$\begin{cases} v(t) = v_0 \\ x(t) = x_0 + v_0 t \end{cases} \tag{54}$$

So now we have a system that fully predicts the position and speed of our electron at any point in time, given some initial position and velocity.

4.2 Quantum Particle

Now we will analyse and model the same problem, using Schrödinger's model for Quantum Mechanics.

In classical mechanics, we made the assumption that the electron occupied a single point in space, and modeled this location by the function $x(t) : \mathbb{R} \to \mathbb{R}^3$. In quantum mechanics, we can not simplify the problem to a single coordinate, instead we model the 'location' of an electron in the form of a wave function $\psi(x) : \mathbb{R}^3 \to \mathbb{C}$, $\psi(x) \in L^2(\mathbb{R}^3)$ that we can use to extrapolate the probability of finding the electron in some space, using the probability distribution function

$$|\psi(x,t)|. \tag{55}$$

The state of the electron however may not be constant, so we would like to track the state of the electron as it changes over time, as we did in the classical model. So we consider time dependent functions, where the wave function at time $t \in \mathbb{R}$ is $\psi(\cdot,t) : \mathbb{R}^3 \to \mathbb{C}$, $\psi(.,t) \in L^2(\mathbb{R}^3)$. We assume to know the state of the electron at some point in time, t_0:

$$\psi(x,t_0) = \psi_0(x). \tag{56}$$

Furthermore, we assume that the function $|\psi_0(x)|^2$ is a probability distribution that predicts where the electron will express itself at time 0. Thus, $\int_{\mathbb{R}^3} |\psi_0(x)|^2 dx = ||\psi_0||^2 = 1$.

In classical mechanics, we used Newton's laws to describe how our system might evolve over time. Now, we use Schrödinger's equation 8 instead. In the case of the free electron, the wave function is not subject to any energy potential, so $V(x) = 0$. The Cauchy-Problem, or initial-value problem of our free electron problem then is

$$\begin{cases} i\hbar \frac{\partial}{\partial t}\psi(x,t) & = -\frac{\hbar^2}{2m}\Delta_x \psi(x,t), \\ \psi(x,t_0) & = \psi_0(x). \end{cases} \tag{57}$$

To find the solution to this Cauchy-Problem, we define the Schrödinger operator of this system H_0:

$$H_0 = -\frac{\hbar^2}{2m}\Delta_x. \tag{58}$$

This linear operator is a scalar multiple of $-\Delta_x$, as such it is an unbounded and self-adjoint linear operator. A proof that $-\Delta_x$ is unbounded and self-adjoint can be found in the mathematical Supplement 6.1.

It follows from the theorem on conservation of probability 3.9 that the evolution equation of the Cauchy-problem then conserves probability, and the *dynamics exist*. Thus for any

solution ψ, $|\psi(.,t)|^2$ functions as a proper probability distribution for any t, describing where the electron can be detected in space at that time. Furthermore, we have seen that for a self adjoint Schrödinger operator, the solution to this Cauchy-problem is the unique solution given by

$$\psi(x,t) = U(t-t_0)\psi_0(x) \tag{59}$$

where $U(t) = e^{-itH_0/\hbar}$.

The solution of the Cauchy-problem 57 is thus a wave function:

$$\psi(x,t) = e^{-\frac{i}{\hbar}(t-t_0)H_0}\psi_0(x) \tag{60}$$

Using the property $U(t)U(s) = U(t+s)$ described in theorem 3.10, we can arbitrarily choose any starting time t_0^*, by considering instead the initial value $\psi_0^* = U(t_0^* - t_0)\psi_{t_0}$. Thus going forward we will for simplicity assume $t_0 = 0$.

Can we find an expression for this function? Although the operator $U(t)$ is well defined, the limit statement is not an expression of our solution in terms of ψ_0. Instead, we would like to find the integral operator form of our solution. To find such an expression we will use Fourier Transforms.

Consider the function

$$g(k) = e^{-\frac{it}{2m\hbar}|k|^2} = \sum_{n=0}^{\infty} \frac{1}{n!}(\frac{it}{2m\hbar}|k|^2)^n \tag{61}$$

where $k \in \mathbb{R}^3$, and $|k|^2$ is $\sum k_i^2$, $i \in \{1,2,3\}$. This function g is called a *Gaussian function*, or simply *Gaussian*.

Then, as we saw in 3.12, we can define the operator $g(p)$, where $p = -i\hbar\nabla_x$, $|p|^2 = -\hbar^2\Delta_x$, using the Fourier transform:

$$\begin{aligned} g(p)\psi(x) = F^{-1}(g(x)F\psi(x)) \text{ so that} \\ g(p) = e^{\frac{-it\hbar}{2m}\Delta_x} \end{aligned} \tag{62}$$

defines the same operator on $\mathcal{D}(\Delta)$ as the operator $U(t)$. Using equation 51, we find that this solution can be expressed as

$$g(p)\psi = (2\pi\hbar)^{-3/2}(F^{-1}g * \psi). \tag{63}$$

The inverse Fourier transform of the Gaussian is known [10, sec 12.3] to be

$$F^{-1}g(x) = (\frac{it}{m})^{-3/2}e^{-\frac{im}{2\hbar t}|x|}.$$

Using equation 63 we are left with the following representation of the solution:

$$\psi(x,t) = U(t)\psi_0(x) = (2\pi\hbar\frac{it}{m})^{-3/2}\int_{\mathbb{R}^3} e^{\frac{im}{2\hbar t}|x-y|^2}\psi_0(y)dy. \tag{64}$$

To conclude this section, we would like to show that under the right circumstances, this wave function has comparable behavior to what we would expect given the classical model. Namely, we point out that if the Fourier transform of the initial condition is *localized* around some point $k_0 \in \mathbb{R}^3$, then our solution is localized around $x = vt$ for some v. We say that a (wave) function is localized around k if there is some small neighborhood, say $B_r(k) = \{x \in \mathbb{R}^3 | |x-k| \leq r\}$ around point k, such that the wave function approaches 0 at an at most exponential rate outside of this neighborhood.

We rewrite equation 64 to show this. Using $|x-y|^2 = |x|^2 - 2(x\cdot y) + |y|^2$, we can split the exponent so that

$$\psi(x,t) = (2\pi\hbar\frac{it}{m})^{-3/2}\int_{\mathbb{R}^3} e^{\frac{im}{2\hbar t}|x|^2}e^{-\frac{im}{\hbar t}(x\cdot y)}e^{\frac{im}{2\hbar t}|y|^2}\psi_0(y)dy.$$

Now we define for $t \in \mathbb{R}\setminus\{0\}$, $\psi_t(y) := e^{i\frac{m|y|^2}{2\hbar t}}\psi(y)$, so that

$$\begin{aligned}\psi(x,t) &= (2\pi\hbar\frac{it}{m})^{-3/2}e^{\frac{im}{2\hbar t}|x|^2}\int_{\mathbb{R}^3} e^{-\frac{i}{\hbar}(\frac{m}{t}x\cdot y)}e^{-\frac{im}{2\hbar t}|y|^2}\psi_0(y)dy \\ &= (\frac{it}{m})^{-3/2}e^{\frac{im}{2\hbar t}|x|^2}F\psi_t(\frac{m}{t}x).\end{aligned} \tag{65}$$

We would like to show that if $F\psi(k)$ is localized around k_0, $F\psi_t(k)$ is also localized around k_0, because then we can clearly see that $\psi(x,t)$ is indeed localized around $k_0 = \frac{m}{t}x$. To show this localization, we show that

$$\psi_t = e^{\frac{im}{2t\hbar}|\cdot|^2}\psi \to \psi \text{ as } t\to\infty. \tag{66}$$

in $L^2(\mathbb{R}^3)$. First we note that $\psi_t(y)$ clearly converges point wise, in fact it converges absolutely,

$$|e^{\frac{im}{2t\hbar}|y|^2}\psi(y) - \psi(y)| = |(e^{\frac{im}{2t\hbar}|y|^2}-1)\psi(y)| \leq |e^{\frac{im}{2t\hbar}|y|^2}-1||\psi(y)| \leq |\psi(y)|. \tag{67}$$

Furthermore, since $|e^{\frac{im}{2t\hbar}|\cdot|^2}| = 1$, we can use the Dominated convergence theorem [6, Thm A.19] to show that

$$\begin{aligned}\lim_{t\to\infty} F\psi_t(k) &= \lim_{t\to\infty}(2\pi\hbar)^{-3/2}\int_{\mathbb{R}^3} e^{-\frac{i}{\hbar}k\cdot x}e^{\frac{im}{2t\hbar}|x|^2}\psi(y)dy \\ &= (2\pi\hbar)^{-3/2}\int_{\mathbb{R}^3} e^{-\frac{i}{\hbar}k\cdot x}\psi(y)dy = F\psi(k),\end{aligned} \tag{68}$$

thus $F\psi_t$ is indeed localized around k_0 for high t. Using this, we can see that the function in equation 65 is localized around $k_0 = \frac{m}{t}x$, or $x = \frac{k_0}{m}t$. Which matches the classical description of a particles evolution, with $v = \frac{k_0}{m}$.

5 Conclusion

In this thesis, we have outlined the basic Schrödinger model of quantum mechanics using mathematical theory, focused specifically on functional analysis and applied this to the problem of a free electron. We began by considering some key physical insights to justify the model in general terms, and then used theory on Hilbert spaces to define the model mathematically. Then we provided an overview the necessary operator theory to describe solutions for the model. Specifically, we noticed that self-adjointness of such operators was a key component in finding such solutions. We used this theory to define solutions in the form of exponentials of operators 3.9. Then we used theory on Fourier transforms to find expressions for such solutions.

Using this overview of the mathematics behind the Schrödinger model of quantum mechanics we attempted to describe the behavior of a free electron and contrast it with the classical view on the behavior of particles. This left us with the expression 64. As discussed, unlike the classical view of particles, the solution to the Schrödinger model came in the form of a wave function, that we use to describe the electron in a probabilistic sense. However, we showed how this description for the free electron could still match our ideas in classical mechanics to some degree.

Sadly, some details have been skipped over in this report. Notably, the equivalence between our used definition of self-adjointness and the prevailing definition in mathematical literature is not proven. Similarly, some complex proofs involving the denseness of $C_c^\infty(\mathbb{R}^3)$ and the definition of $L^2(\mathbb{R}^3)$ have been only touched on. Luckily, interested readers can find more information to these issues in our frequently used sources [6][8][7]. We have also avoided using Spectral theory, which severely limits what this thesis can cover. We refer to [4][6][8] for an in-depth look at this theory.

6 Mathematical Supplement

Lemma 6.1. *The Laplacian operator is symmetrical on $C_c^\infty(\mathbb{R}^3)$, and has a unique self-adjoint closure on $L^2(\mathbb{R}^3)$. We say that the Laplacian operator is essentially self adjoint.*

Proof. This proof roughly follows the work of [11]. First we will prove that the Laplacian is symmetrical on $C_c^\infty(\mathbb{R}^3)$, so we prove that, for any $\psi, \phi \in \mathcal{D}(\Delta)$:

$$\langle \Delta\psi, \phi \rangle = \langle \psi, \Delta\phi \rangle.$$

Let $\phi, \psi \in C_c^\infty(\mathbb{R}^3)$. As they are both compactly supported, $\exists U \subset \mathbb{R}^3$ an open subset, with smooth bounds, s.t. ϕ, ψ are 0 on U^c, the compliment of U. Their derivatives are also 0 on U^c.

Applying Green's First Identity [10, 7.1], to $\psi, \overline{\phi}$, we know that

$$\int_U \psi(x)\Delta\overline{\phi(x)} + \nabla\psi(x) \cdot \nabla\overline{\phi(x)}dx = \int_{\partial U} \psi(s)(\nabla\overline{\phi(s)} \cdot \vec{n})ds, \tag{69}$$

where ∂U is the boundary set of U, $\vec{n}$ is a directed normal vector.

This is effectively integration by parts in higher dimensions. Notice however that ϕ, ψ and their derivatives are explicitly 0 on ∂U, and as a result, the integral on the right equals 0. As a result, we find that for our functions ψ, ϕ

$$\int_U \psi(x)\Delta\overline{\phi(x)} + \nabla\psi(x) \cdot \nabla\overline{\phi(x)}dx = 0.$$

Applying this same trick twice, we see that,

$$\int_U \psi(x)\Delta\overline{\phi(x)}dx = -\int_U \nabla\psi(x) \cdot \nabla\overline{\phi(x)}dx = \int_U \Delta\psi(x)\overline{\phi(x)}dx.$$

Since we have defined ψ and ϕ to both be equivalent to 0 outside of the set U, these statements imply that

$$\int_{\mathbb{R}^3} \psi(x)\Delta\overline{\phi(x)}dx = \int_{\mathbb{R}^3} \Delta\psi(x)\overline{\phi(x)}dx.$$

Using the fact that $\Delta\overline{\phi} = \overline{\Delta\phi}$, this proves symmetry of the Laplacian on $C_c^\infty(\mathbb{R}^3)$.

Now that we have proven that the Laplacian on $C_c^\infty(\mathbb{R}^3)$ is symmetric, we can use the Closure theorem for symmetric operators 3.7 to show that there is a symmetric closed operator that extends this Laplacian. Unless specified otherwise, as we do in this proof, when refer to the Laplacian on $\mathcal{D}(\Delta) \subset L^2(\mathbb{R}^{\not 4})$, this closure is what we refer to. To prove our lemma, we need to show that this closed operator is self-adjoint. This proof comes in

two parts, first we need to show that there is for any sequence $(\phi_n) \subset C_c^\infty(\mathbb{R}^3)$,

$$(\Delta + i)\phi_n \to \psi \tag{70}$$

implies that ϕ_n converges to some ϕ in $L^2(\mathbb{R}^3)$. Then, since Δ is closed, $(\Delta + i)\phi = \psi$.

Second, we need to prove that the range of the Laplacian on $C_c^\infty(\mathbb{R}^3)$ is dense in $L^2(\mathbb{R}^3)$, so that such a convergent sequence exists for every element of $L^2(\mathbb{R}^3)$.

Let some sequence $(\phi_n) \subset C_c^\infty(\mathbb{R}^3)$, such that

$$(\Delta + i)\phi_n \to \psi \tag{71}$$

as $n \to \infty$. Then ϕ_n is Cauchy and for $m > n$,

$$||(\Delta + i)(\phi_n - \phi_m)|| \to 0$$

as $n, m \to \infty$. Using that Δ is symmetric, we can show that

$$\begin{aligned} ||(\Delta + i)(\phi_n - \phi_m)||^2 &= \langle (\Delta + i)(\phi_n - \phi_m), (\Delta + i)(\phi_n - \phi_m)\rangle \\ &= \langle (\Delta - i)(\Delta + i)(\phi_n - \phi_m), (\phi_n - \phi_m)\rangle \\ &= \langle (\Delta^2 + 1)(\phi_n - \phi_m), (\phi_n - \phi_m)\rangle \\ &= ||\Delta(\phi_n - \phi_m)||^2 + ||\psi_n - \psi_m||^2 \to 0, \end{aligned}$$

and thus indeed $||\psi_n - \psi_m||^2 \to 0$, thus (ψ_n) is Cauchy and converges in $L^2(\mathbb{R}^3)$.

To prove that the range of the Laplacian on $C_c^\infty(\mathbb{R}^3)$ is dense in $L^2(\mathbb{R}^3)$, we show that its orthogonal complement is $\{0\}$, or equivalently, that for $\phi \in C_c^\infty(\mathbb{R}^3)$,

$$\langle \phi, (\Delta + i)\psi\rangle = 0 \text{ for all } \psi \in C_c^\infty(\mathbb{R}^3) \implies \phi = 0. \tag{72}$$

Consider such a ϕ, then by the symmetry of the Laplacian,

$$\langle \phi, (\Delta + i)\psi\rangle = \langle (\Delta - i)\phi, \psi\rangle = 0 \tag{73}$$

for all $\psi \in C_c^\infty(\mathbb{R}^3)$. By equivalence, we know that $(\Delta - i)\phi = 0$, and thus $i\phi = \Delta\phi$. Using the Fourier transform (3.11), we can see that this is only possible for $\phi = 0$, since the system

$$\begin{aligned} F(z\phi)(x) &= zF\phi(x) \\ F(\Delta\phi)(x) &= -\frac{1}{\hbar^2}|x|^2 F\phi(x) \end{aligned}$$

only has the solution $\phi = 0$. □

Lemma 6.2. *For any unbounded self-adjoint operator A, the family of operators defined by*

$$A_\lambda := \frac{1}{2}\lambda^2 \left((A + i\lambda)^{-1} + (A - i\lambda)^{-1}\right) \text{ for } \lambda > 0, \tag{74}$$

for $\lambda \in \mathbb{R}$, $\lambda \neq 0$, are bounded operators such that

$$A_\lambda \to A \text{ as } \lambda \to \infty. \tag{75}$$

Proof. To prove this, we will construct some B_λ, such that $A_\lambda = B_\lambda A$ on $\mathcal{D}(A)$. Then, by showing that $B_\lambda \to I$ as $\lambda \to \infty$, we prove our initial claim.

Let A a self-adjoint operator, then $\mathcal{R}(A + i\lambda) = \mathcal{H}$ for any $\lambda \in \mathbb{R}$, $\lambda \neq 0$, where $\mathcal{H}$ is some hilbert space. Then, for any $\phi \in \mathcal{D}(A)$, we can find some $\psi_1, \psi_2 \in \mathcal{H}$, such that

$$\begin{cases} (A + i\lambda)\psi_1 = A\phi \\ (A - i\lambda)\psi_2 = A\phi. \end{cases} \tag{76}$$

We can solve for ψ_1 and ψ_2 in this equation using two slightly different methods. Firstly, since the resolvent operator exists and is bounded and linear (3.7), we can see that

$$\begin{cases} \psi_1 = (A + i\lambda)^{-1} A\phi \\ \psi_2 = (A - i\lambda)^{-1} A\phi, \end{cases} \tag{77}$$

and thus we find that

$$(\psi_1 - \psi_2) = \left((A + i\lambda)^{-1} - (A - i\lambda)^{-1}\right) A\phi. \tag{78}$$

Alternatively, we can solve the equations 76 for ψ_1, ψ_2 as follows. First we consider for ψ_2 that,

$$(A - i\lambda)\psi_2 = A\phi - i\lambda\phi + i\lambda\phi = (A - i\lambda)\phi + i\lambda\phi,$$

and again using the resolvent operator (3.7), we see that

$$\psi_2 = \phi + (A - i\lambda)^{-1} i\lambda\phi = \phi + i\lambda(A - i\lambda)^{-1}\phi. \tag{79}$$

Similarly, we can show that

$$\psi_1 = \phi - i\lambda(A + i\lambda)^{-1}\phi. \tag{80}$$

Combining equations 80 and 79 we can find an second equality,

$$\psi_1 - \psi_2 = -i\lambda \left((A + i\lambda)^{-1} + (A - i\lambda)^{-1}\right) \phi, \tag{81}$$

which, comparing it to our definition of A_λ, implies that

$$A_\lambda \phi = \frac{1}{2} i\lambda(\psi_1 - \psi_2). \tag{82}$$

Plugging our first equation 78 into this equality, we find that

$$A_\lambda \phi = \frac{1}{2} i\lambda(\psi_1 - \psi_2) = \frac{1}{2} i\lambda \left((A + i\lambda)^{-1} - (A - i\lambda)^{-1} \right) A\phi. \tag{83}$$

Thus we construct the operator

$$B_\lambda := \frac{1}{2} i\lambda \left((A + i\lambda)^{-1} - (A - i\lambda)^{-1} \right), \tag{84}$$

such that $A_\lambda = B_\lambda A$.

Now we would like to show that this $B_\lambda \to I$ as $\lambda \to \infty$ on $\mathcal{D}(A)$.

Using the equations 79, 80, we now consider,

$$\begin{aligned} \frac{1}{2}(\psi_1 + \psi_2) =& \frac{1}{2} \left(2\phi - i\lambda(A + i\lambda)^{-1}\phi + i\lambda(A + i\lambda)^{-1}\phi \right) \\ &= I\phi - B_\lambda \phi = (I - B_\lambda)\phi, \end{aligned}$$

which tells us that if $\psi_1 + \psi_2$ converges to 0, B_λ indeed converges to I on $\mathcal{D}(A)$. We consider $\psi_1 + \psi_2$ using equations 77, to find

$$\frac{1}{2}(\psi_1 + \psi_2) = \frac{1}{2} \left((A + i\lambda)^{-1} + (A - i\lambda)^{-1} \right) A\phi,$$

which is easier to evaluate as $\lambda \to \infty$. Using the upper bound for the resolvent operator 16, we find that

$$||(I - B_\lambda)\phi|| = ||\frac{1}{2} \left((A + i\lambda)^{-1} + (A - i\lambda)^{-1} \right) A\phi|| \leq \frac{1}{|\lambda|} ||A\psi|| \to 0 \tag{85}$$

as $\lambda \to \infty$, proving the lemma. □

Lemma 6.3. *Let A an unbounded linear operator, then the family of operators*

$$e^{iA} := \lim_{\lambda \to \infty} e^{iA_\lambda} \tag{86}$$

, where A_λ is defined by 17 is well-defined.

Proof. We prove this lemma by showing that e^{iA_λ} is a cauchy family, meaning that

$$||e^{iA_\lambda} - e^{iA_{\lambda'}}|| \to 0 \text{ as } \lambda, \lambda' \to \infty,\ \lambda' > \lambda. \tag{87}$$

We begin by recognising that e^{iA_λ} is an operator that satisfies the properties outlined in theorem 3.10, up to the use of a constant $\hbar$, thus satisfying properties 22 and 24. As such we can use the fundamental theorem of calculus to show that

$$e^{iA'_\lambda}\psi - e^{iA_\lambda}\psi = \int_0^1 \frac{\partial}{\partial s} e^{isA_{\lambda'}} e^{i(1-s)A_\lambda} ds,$$

and using the chain rule

$$e^{iA'_\lambda}\psi - e^{iA_\lambda}\psi = \int_0^1 (iA_{\lambda'} - iA_\lambda) e^{isA_{\lambda'}} e^{i(1-s)A_\lambda}\psi ds.$$

To evaluate the limit of this family, we consider

$$\begin{aligned} ||e^{iA_\lambda} - e^{iA_{\lambda'}}\psi||^2 &= || \int_0^1 e^{isA_\lambda} e^{i(1-s)A_{\lambda'}} i(A_\lambda - A_{\lambda'})\psi ds||^2 \\ &\leq \int_0^1 ||e^{isA_\lambda} e^{i(1-s)A_{\lambda'}} i(A_\lambda - A_{\lambda'})\psi||^2 ds. \end{aligned} \tag{88}$$

This inequality holds, because the norm on the right hand side is continuous over time, as we have seen proving theorem 3.10 for bounded operators, and thus is Riemann integrable in s. We will show that the inequality is true below. Consider

$$f(s,x) = e^{isA_\lambda} e^{i(1-s)A_{\lambda'}} i(A_\lambda - A_{\lambda'})\psi(x),$$

then

$$\int_{\mathbb{R}^3} | \int_0^1 f(s,x) ds|^2 dx \leq \int_{\mathbb{R}^3} \int_0^1 |f(s,x)|^2 ds dx = \int_0^1 \int_{\mathbb{R}^3} |f(s,x)|^2 dx ds = \int_0^1 ||f(s,.)|| ds.$$

Proving the inequality in equation 88.

Furthermore, since e^{iA_λ} meets the property of equation 25 in theorem 3.10,

$$\begin{aligned} ||e^{iA_\lambda} - e^{iA_{\lambda'}}\psi||^2 &\leq \int_0^1 ||e^{isA_\lambda} e^{i(1-s)A_{\lambda'}} i(A_\lambda - A_{\lambda'})\psi||^2 ds = \int_0^1 ||(A_\lambda - A_{\lambda'})\psi||^2 ds \\ &= ||(A_\lambda - A_{\lambda'})\psi||^2. \end{aligned} \tag{89}$$

We have shown in lemma 6.2 that A_λ indeed converges on $\mathcal{D}A$, thus e^{iA_λ} also converges on this domain, proving the lemma. □

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