# The Schrödinger Equation

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## Introduction

The Schrödinger equation arose out of a need to explain phenomena in physics, such as energy quantization and wave-particle duality. It can be thought of as an analogue to Newton's second law in that in classical mechanics, we may obtain the position $x(t)$ of a non-relativistic particle of mass $m$ subject to a force by solving Newton's second law, whereas in quantum mechanics, we may solve the Schrödinger equation to obtain a nonrelativistic particle's wave function which can provide us with a quantity that nearly resembles the particle's position.

In the first section, I discuss the four main axioms on which quantum mechanics is built upon. In the second section, I show that the operators which correspond to observables are self-adjoint. In the third section, I define a functional calculus for self-adjoint operators which is necessary for an understanding of the fourth section; any results stated in this section are done so without proof. In the fourth section, I discuss the time evolution of the Schrödinger equation.

The first two sections closely follow [2] while the last two sections closely follow [1].

## Axioms of Quantum Mechanics

In quantum mechanics, a particle in $\mathbb{R}^3$ is described by a complex-valued function called the wave function: $\psi(x,t)$ where $(x,t) \in \mathbb{R}^3 \times \mathbb{R}$ and as usual, $x$ is position and $t$ is time. Given a general quantum mechanical system, we say that its state is $\psi(x,t)$.

These wave functions live inside a complex Hilbert space $\mathcal{H}$. The norm $||\psi||$ of $\psi \in \mathcal{H}$ is given by,

$$||\psi||^2 = \langle \psi, \psi \rangle = \int_{\mathbb{R}^3} \psi^* \psi = \int_{\mathbb{R}^3} |\psi(x,t)|^2 d^3x.$$

We interpret the wave function as a probability: specifically, at a given time $t$, it provides us with a probability density $|\psi(x,t)|^2$ for the particle. From this, we can determine the probability of finding the particle in a region $V$, at a given time $t$, by calculating

$$\int_V |\psi(x,t)|^2 d^3x. \tag{1}$$

Then we should obviously have,

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

as the particle must be somewhere in space. Thus, wave functions must be normalized so that (2) holds true. This requirement can be simply stated as $||\psi|| = 1$.

Collecting most of the above statements, we can state the first axiom.

**Axiom 1**: Wave functions $\psi$ live in a complex Hilbert space $\mathcal{H}$ and they must satisfy $||\psi|| = 1$.

To get started on the second axiom, let us return to (1). Observe that with the characteristic function $\chi_V$, we can write this as,

$$\langle \psi, \chi_V \psi \rangle = \langle \chi_V \psi, \psi \rangle = \int_{\mathbb{R}^3} \chi_V |\psi(x,t)|^2 d^3x = \int_V |\psi(x,t)|^2 d^3x, \tag{3}$$

and the position of the particle $x$ can be calculated by,

$$\langle \psi, x\psi \rangle = \langle x\psi, \psi \rangle = \int_{\mathbb{R}^3} x|\psi(x,t)|^2, \tag{4}$$

though it is important to note that due to the probabilistic interpretation, the position $x$ of the particle is a random variable and so (4) is actually the expectation value of $x$: that is, it represents the average of measuring the location, at $x$, of many particles where each particle is described by the same wave function $\psi(x,t)$.

Now, physical quantities that can be measured (like position, momentum, and energy) are referred to as observables. Examining (3) and (4), we get the sense that observables correspond to linear operators. This is the statement of the second axiom.

**Axiom 2**: Each observable $a$ corresponds to a linear operator $A : \mathcal{D}_A \longrightarrow \mathcal{H}$ where $\mathcal{D}_A$ is a dense subset of $\mathcal{H}$; this operator is defined maximally.

The operator $A$ being defined maximally means the following: If there is another operator $\tilde{A}$ such that $A \subseteq \tilde{A}$ (which means $\mathcal{D}_A \subseteq \mathcal{D}_{\tilde{A}}$ and $A\psi = \tilde{A}\psi \ \forall \psi \in \mathcal{D}_A$), then $A = \tilde{A}$. The operator $\tilde{A}$ is called the extension of $A$.

Note that in general, given an observable, there is no procedure for determining the corresponding linear operator.

**Remark.** *As we shall see in the next section, the operators which correspond to observables are symmetric. By the Hellinger-Toeplitz theorem, a symmetric operator defined on the entire Hilbert space is bounded, but in quantum mechanics it is certainly possible for our operators to be unbounded, thus we require that our operators $A$ only be defined on $\mathcal{D}_A$ (it is dense for the reason of wanting $A$ to be defined on most of the Hilbert space).*

*The proof of the Hellinger-Toeplitz theorem is a consequence of the closed graph theorem: One can show that if $A$ is symmetric and defined on all of $\mathcal{H}$, then it is closed and so, by the closed graph theorem, it is bounded.*

Given that an observable is a physical quantity that may be measured, we require that its expectation value, which we denote as $\langle A \rangle$, is a real number. This leads to the third axiom.

**Axiom 3**: Given an observable $a$ whose linear operator is $A$, its expectation value $\langle A \rangle = \langle \psi, A\psi \rangle = \langle A\psi, \psi \rangle$ must be a real number.

The fourth axiom concerns the time evolution of a quantum mechanical system. If we are given an initial state of the system, denoted simply as $\psi(0)$, then at time $t$, there should be a unique $\psi(t)$ representing the state of the system. We write this relation as

$$\psi(t) = U(t)\psi(0)$$

where $U(t)$ is an operator $U : \mathbb{R} \times \mathcal{H} \longrightarrow \mathcal{H}$. Experiments done in physics shows that the superposition of states is valid, meaning the following is true:

$$U(t)(c_1\psi_1(0) + c_2\psi_2(0)) = c_1\psi_1(t) + c_2\psi_2(t).$$

Then by the above, $U(t)$ should be a linear operator. Furthermore, our requirement that $||\psi(t)|| = 1$ for all $t$ means that

$$||U(t)\psi|| = ||\psi||$$
$$\Rightarrow \langle U(t)\psi, U(t)\psi \rangle = \langle \psi, \psi \rangle .$$

Thus, $U(t)$ is a unitary operator. We should also have

$$U(0) = \mathbb{I}, \qquad U(t+s) = U(t)U(s) \tag{5}$$

where $\mathbb{I}$ is just the identity operator.

**Definition.** *A one-parameter unitary group on a Hilbert space $\mathcal{H}$ is a family of unitary operators $U(t)$, $t \in \mathbb{R}$ , with the properties,*

*(i)* $U(0) = \mathbb{I}$

*(ii)* $U(s+t) = U(s)U(t)$ *for all* $s, t \in \mathbb{R}$.

*A one-parameter unitary group is said to be strongly continuous if*

$$\lim_{s \to t} ||U(t)\psi - U(s)\psi|| = 0,$$

*for all $\psi \in \mathcal{H}$ and all $t \in \mathbb{R}$.*

**Definition.** *If $U(\cdot)$ is a strongly continuous one-parameter unitary group, the infinitesimal generator of $U(\cdot)$ is the operator $A$ given by,*

$$A\psi = \lim_{t \to 0} \frac{1}{i} \frac{U(t)\psi - \psi}{t}, \tag{6}$$

*where $\mathcal{D}_A$, the domain of $A$, consists of the $\psi \in \mathcal{H}$ for which this limit exists.*

The above definitions lead us to the last axiom.

**Axiom 4**: The time evolution of a wave function is given by a strongly continuous one-parameter unitary group $U(t)$, $t \in \mathbb{R}$; the infinitesimal generator $H$ of this group is the operator which corresponds to the energy of the system; thus, this operator is called the Hamiltonian.

Now if $\psi(0) \in \mathcal{D}_H$, then (6) becomes

$$-i\frac{d}{dt}\psi(t) = H\psi(t) \tag{7}$$

and $\psi(t)$ is a solution to this equation. With appropriate constants, (7) is the Schrödinger equation.

For example, if the energy $E$ of a particle moving in $\mathbb{R}$ was given by

$$E = \frac{p^2}{2m} + V(x),$$

where $V(x)$ is the potential energy function and $p$ is momentum, then our Hamiltonian operator would be given by,

$$H = \frac{P^2}{2m} + V(X),$$

where $P = -i\hbar\frac{d}{dx}$ and $X = x$ are, respectively, the operators corresponding to the momentum $p$ and position $x$. Then (7), with a factor of $-\hbar^{-1}$, would become,

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

## Observables Correspond to Self-adjoint Operators

**Definition.** *A densely defined linear operator $A$ is called symmetric if*

$$\langle\varphi, A\psi\rangle = \langle A\varphi, \psi\rangle, \qquad \psi, \varphi \in \mathcal{D}_A$$

**Lemma 1.** *A densely defined operator $A$ is symmetric if and only if $\langle\psi, A\psi\rangle$ is real-valued for all $\psi \in \mathcal{D}_A$.*

*Proof.* If $A$ is symmetric, then,

$$\langle\psi, A\psi\rangle = \langle A\psi, \psi\rangle = \langle\psi, A\psi\rangle^*$$

which implies that $\mathrm{Im}(\langle\psi, A\psi\rangle) = 0$ for all $\psi \in \mathcal{D}_A$.

For the other direction, consider $\langle\psi + i\varphi, A(\psi + i\varphi)\rangle$ to get the following identity:

$$\begin{aligned}\langle\psi + i\varphi, A(\psi + i\varphi)\rangle &= \langle\psi + i\varphi, A\psi\rangle + i\,\langle\psi + i\varphi, A\varphi\rangle \\ &= \langle\psi, A\psi\rangle + \langle\varphi, A\varphi\rangle + i(\langle\psi, A\varphi\rangle - \langle\varphi, A\psi\rangle)\end{aligned}$$

By our assumption, the imaginary part should be zero, that is, the real part of what is contained in the parenthesis should be zero: $\mathrm{Re}\langle\varphi, A\psi\rangle = \mathrm{Re}\langle\psi, A\varphi\rangle = \mathrm{Re}\langle A\varphi, \psi\rangle$. Thus, we have shown symmetry of the real part of $\langle\varphi, A\psi\rangle$. Now simply replace $\varphi$ with $i\varphi$ to get:

$$\begin{aligned} Re(-i\,\langle\varphi, A\psi\rangle) &= Re(-i\,\langle A\varphi, \psi\rangle) \\ \Leftrightarrow Im(\langle\varphi, A\psi\rangle) &= Im(\langle A\varphi, \psi\rangle). \end{aligned}$$

So we now have symmetry of the imaginary part as well. Thus, $A$ is symmetric because we have $\langle\varphi, A\psi\rangle = \langle A\varphi, \psi\rangle$.

□

**Remark.** *Given Lemma 1 and Axiom 3, we conclude that all operators which correspond to observables must be symmetric.*

We now define the adjoint of an operator. Recall that in the case where $A : \mathcal{H} \longrightarrow \mathcal{H}$ is a bounded linear operator, the adjoint, $A^*$, is defined by,

$$\langle\varphi, A^*\psi\rangle = \langle A\varphi, \psi\rangle\,.$$

However, in our case we may have $A$ unbounded and so we have the following definition for the adjoint operator.

**Definition.** *The adjoint operator $A^*$ of a densely defined linear operator $A$ is defined by,*

$$\begin{aligned} A^* : \mathcal{D}_{A^*} &\longrightarrow \mathcal{H} \\ \psi &\longmapsto \tilde{\psi} \end{aligned}$$

*where* $\mathcal{D}_{A^*} = \{\, \psi \in \mathcal{H} \,|\, \exists\tilde{\psi} \in \mathcal{H} \,:\, \langle\psi, A\varphi\rangle = \langle\tilde{\psi}, \varphi\rangle\,, \forall\varphi \in \mathcal{D}_A \,\}$.

**Definition.** *If $A = A^*$, the operator $A$ is called self-adjoint.*

To ease the process of determining if an operator $A$ is self-adjoint, we have the following lemma.

**Lemma 2.** *Let $A$ be symmetric such that $Ran(A + z) = Ran(A + z^*) = \mathcal{H}$ for one $z \in \mathbb{C}$, where Ran refers to range. Then $A$ is self-adjoint.*

*Proof.* Let $\psi \in \mathcal{D}_{A^*}$ so that $A^*\psi = \tilde{\psi}$. Since we assume that $\mathrm{Ran}(A + z^*) = \mathcal{H}$, there must be a $\rho \in \mathcal{D}_A$ such that $(A + z^*)\rho = \tilde{\psi} + z^*\psi$. Now for any $\varphi \in \mathcal{D}_A$, we have,

$$\begin{aligned} \langle\psi, (A + z)\varphi\rangle &= \langle\psi, A\varphi\rangle + \langle\psi, z\varphi\rangle \\ &= \langle\tilde{\psi}, \varphi\rangle + \langle z^*\psi, \varphi\rangle \\ &= \langle\tilde{\psi} + z^*\psi, \varphi\rangle \\ &= \langle(A + z^*)\rho, \varphi\rangle \\ &= \langle A\rho, \varphi\rangle + \langle z^*\rho, \varphi\rangle \\ &= \langle\rho, A\varphi\rangle + \langle\rho, z\varphi\rangle \\ &= \langle\rho, (A + z)\varphi\rangle \end{aligned}$$

and since $\text{Ran}(A+z) = \mathcal{H}$ we may conclude that $\psi = \rho \in \mathcal{D}_A$. Thus, $(A+z^*)\rho = \tilde{\psi} + z^*\psi$ implies $A\psi = \tilde{\psi} = A^*\psi$, and so $A$ is indeed self-adjoint.

□

We say that a densely defined operator is nonnegative (resp. positive) if $\langle \psi, A\psi \rangle \geq 0$ (resp. $> 0$ for $\psi \neq 0$) for all $\psi \in \mathcal{D}_A$.

**Remark.** *By Lemma 1, a nonnegative operator is symmetric.*

Given a nonnegative operator $A$ we may define a scalar product on $\mathcal{D}_A$ as

$$\langle \varphi, \psi \rangle_A = \langle \varphi, (A+1)\psi \rangle .$$

Observe that $||\psi|| \leq ||\psi||_A$. Now let $\mathcal{H}_A$ be the completion of $\mathcal{D}_A$ with respect to this scalar product. Though it shall not be proven here, it can be shown that $\mathcal{D}_A \subseteq \mathcal{H}_A \subseteq \mathcal{H}$.

**Lemma 3.** *Suppose $A$ is a nonnegative operator. Then there is a nonnegative extension $\tilde{A}$, given by restricting $A^*$ to $\mathcal{H}_A$, such that $Ran(\tilde{A}+1) = \mathcal{H}$.*

*Proof.* Define the operator $\tilde{A}$ by,

$$\begin{aligned} \tilde{A} : \mathcal{D}_{\tilde{A}} &\longrightarrow \mathcal{H} \\ \psi &\longmapsto \tilde{\psi} - \psi \end{aligned}$$

where $\mathcal{D}_{\tilde{A}} = \{ \psi \in \mathcal{H}_A \,|\, \exists \tilde{\psi} \in \mathcal{H} : \langle \varphi, \psi \rangle_A = \langle \varphi, \tilde{\psi} \rangle , \forall \varphi \in \mathcal{H}_A \}$.

First, let us see how $\tilde{A}$, as defined above, is a restriction of $A^*$ to $\mathcal{H}_A$. Consider an arbitrary $\psi \in \mathcal{D}_{\tilde{A}}$; then for all $\varphi \in \mathcal{H}_A$, we have,

$$\begin{aligned} \langle \varphi, \tilde{\psi} \rangle &= \langle \varphi, \psi \rangle_A \\ &= \langle \varphi, A\psi \rangle + \langle \varphi, \psi \rangle \\ \Rightarrow \langle \varphi, \tilde{\psi} - \psi \rangle &= \langle \varphi, A\psi \rangle \\ &= \langle A\varphi, \psi \rangle . \end{aligned}$$

Then because this holds $\forall \varphi \in \mathcal{D}_A \subseteq \mathcal{H}_A$, we have $\langle \varphi, \tilde{\psi} - \psi \rangle = \langle A\varphi, \psi \rangle = \langle \varphi, A^*\psi \rangle$ and hence, $\tilde{A}\psi = A^*\psi = \tilde{\psi} - \psi$ for $\psi \in \mathcal{D}_{\tilde{A}}$.

Now, recall that for $\tilde{A}$ to be an extension of $A$, we must have that $\mathcal{D}_A \subseteq \mathcal{D}_{\tilde{A}}$ and $A\psi = \tilde{A}\psi$, $\forall \psi \in \mathcal{D}_A$.

(i) Consider $\psi \in \mathcal{D}_A$. By $\mathcal{D}_A \subseteq \mathcal{H}_A$, we already have $\psi \in \mathcal{H}_A$. Also, because $\psi \in \mathcal{D}_A$, we have that $(A+1)\psi \in \mathcal{H}$ exists; thus $\langle \varphi, \psi \rangle_A = \langle \varphi, \tilde{\psi} \rangle$ holds for all $\varphi \in \mathcal{H}_A$, where for this case we have defined $\tilde{\psi} := (A+1)\psi$.

(ii) Consider an arbitrary $\psi \in \mathcal{D}_A$ (and hence, $\psi \in \mathcal{D}_{\tilde{A}}$). Then for all $\varphi \in \mathcal{D}_A$, we have,

$$\begin{aligned} \langle \varphi, \tilde{A}\psi \rangle &= \langle \varphi, A^*\psi \rangle \\ &= \langle \varphi, \tilde{\psi} \rangle - \langle \varphi, \psi \rangle \\ &= \langle \varphi, \psi \rangle_A - \langle \varphi, \psi \rangle \\ &= \langle \varphi, (A+1)\psi \rangle - \langle \varphi, \psi \rangle \\ &= \langle \varphi, A\psi \rangle , \end{aligned}$$

where in the third line we used the fact that $\mathcal{D}_A$ is dense in $\mathcal{H}_A$. Then from the above calculation, and the fact that $\psi$ was arbitrary, we have that $A\psi = \tilde{A}\psi$, $\forall \psi \in \mathcal{D}_A$.

Next, let us see how $\tilde{A}$ is nonnegative. Consider an arbitrary $\psi \in \mathcal{D}_{\tilde{A}}$. Then,

$$\begin{aligned} \langle \psi, \tilde{A}\psi \rangle &= \langle \psi, \tilde{\psi} \rangle - \langle \psi, \psi \rangle \\ &= \langle \psi, \psi \rangle_A - \langle \psi, \psi \rangle \\ &= \langle \psi, A\psi \rangle \geq 0. \end{aligned}$$

Lastly, let us show that $\text{Ran}(\tilde{A}+1) = \mathcal{H}$. For an arbitrary $\tilde{\psi} \in \mathcal{H}$, we get a bounded linear functional on $\mathcal{H}_A$ defined by $\varphi \longmapsto \langle \tilde{\psi}, \varphi \rangle$. Indeed it is bounded, for by Cauchy-Schwarz, $|\langle \tilde{\psi}, \varphi \rangle| \leq ||\tilde{\psi}|| \cdot ||\varphi|| \leq ||\tilde{\psi}|| \cdot ||\varphi||_A$. Since this linear functional is bounded, it is continuous and thus we may apply the Riesz representation theorem to find a $\psi \in \mathcal{H}_A$ such that $\langle \tilde{\psi}, \varphi \rangle = \langle \psi, \varphi \rangle_A$ for all $\varphi \in \mathcal{H}_A$. Then observe that,

$$\begin{aligned} \langle \psi, \varphi \rangle_A &= \langle \tilde{\psi}, \varphi \rangle \\ \Rightarrow \langle \psi, \varphi \rangle_A^{\;*} &= \langle \tilde{\psi}, \varphi \rangle^* \\ \Leftrightarrow \langle (A+1)\varphi, \psi \rangle &= \langle \varphi, \tilde{\psi} \rangle \\ \Leftrightarrow \langle \varphi, \psi \rangle_A &= \langle \varphi, \tilde{\psi} \rangle . \end{aligned}$$

where in the last line we used the fact that because $A$ is nonnegative it is symmetric. Since this holds for all $\varphi \in \mathcal{H}_A$, we have that $\psi \in \mathcal{D}_{\tilde{A}}$ and thus by the definition of $\tilde{A}$ we have $(\tilde{A}+1)\psi = \tilde{\psi}$ and since $\tilde{\psi} \in \mathcal{H}$ was arbitrary, $\tilde{A}+1$ is surjective and thus $\text{Ran}(\tilde{A}+1) = \mathcal{H}$. □

**Technicality**: Recall that the statement of the Riesz representation theorem is the following: Let $\mathcal{H}$ be a Hilbert space and $\mathcal{H}^*$ be its dual, which is defined as the space of continuous linear functionals on $\mathcal{H}$. Then for any $f \in \mathcal{H}^*$, there exists a unique $\varphi \in \mathcal{H}$ such that $f(\psi) = \langle \varphi, \psi \rangle$ for all $\psi \in \mathcal{H}$.

Now at last, let us return to observables. Let $A$ be an operator corresponding to an observable (recall that this means that $A$ is symmetric). It may certainly not be the case that $A$ is nonnegative, but $A^2$ will most definitely be nonnegative and thus by Lemma 3, it has a nonnegative extension $\tilde{A}^2$ with $\text{Ran}(\tilde{A}^2+1) = \mathcal{H}$. By Axiom 2, we require that $A^2$ be defined maximally and thus $A^2 = \tilde{A}^2$. This also means that $\text{Ran}(A^2+1) = \mathcal{H}$, which in turn allows us to state that for every $\varphi \in \mathcal{H}$, there is a $\psi \in \mathcal{D}_{A^2}$ such that,

$$(A-i)(A+i)\psi = (A+i)(A-i)\psi = \varphi.$$

So $(A \pm i)\psi \in \mathcal{D}_A$ from which we get that $\text{Ran}(A \pm i) = \mathcal{H}$. Then by Lemma 2, $A$ is self-adjoint.

So, we have shown that the operators which correspond to observables are indeed self-adjoint.

## Functions of Self-adjoint Operators

From looking at the Schrödinger equation, it is not difficult to see that the solution could possibly take the form of $e^{itH}\psi(0)$. However, taking the exponential of, or more generally, defining a function of, an operator is a delicate matter.

If our Hilbert space were finite dimensional, $\mathcal{H} = \mathbb{C}^n$, then $H$ could be thought of as a matrix, meaning the Schrödinger equation is nothing but a system of ordinary differential equations. In this case, $e^{itH}$ can be defined by a convergent power series,

$$e^{itH} = \sum_{n=0}^{\infty} \frac{(it)^n}{n!} H^n.$$

For the more common case where $H$ is unbounded, convergence of the power series becomes tricky. It is better to take a different approach, through the spectral theorem for self-adjoint operators. For the sake of brevity, the results in this section will be presented without proof, though they can all be found in [1].

**Definition.** *A projection on a vector space $V$ is a linear map $P : V \longrightarrow V$ such that $P^2 = P$. If $P$ is a Hilbert space, then $P$ is said to be an orthogonal projection if $\langle Px, y\rangle = \langle x, Py\rangle$ for all $x, y \in V$ (thus, $P^* = P$; orthogonal projections are self-adjoint).*

**Definition.** *Let $\mathcal{B}$ be the Borel sigma algebra of $\mathbb{R}$ and $\mathcal{L}(\mathcal{H})$ be the set of bounded linear operators from $\mathcal{H}$ to $\mathcal{H}$. Then a projection-valued measure is a map,*

$$\begin{aligned} \mu : \mathcal{B} &\longrightarrow \mathcal{L}(\mathcal{H}) \\ \Omega &\longmapsto \mu(\Omega) \end{aligned}$$

*such that,*

*(i) For $\Omega \in \mathcal{B}$, $\mu(\Omega)$ is an orthogonal projection.*

*(ii) $\mu(\mathbb{R}) = \mathbb{I}$ and $\mu(\emptyset) = 0$.*

*(iii) If $\Omega = \cup_n \Omega_n$, with $\Omega_m \cap \Omega_n = \emptyset$ for $n \neq m$, then $\sum_n \mu(\Omega_n)\psi = \mu(\Omega)\psi$ for every $\psi \in \mathcal{H}$.*

*(iv) $\mu(\Omega_1)\mu(\Omega_2) = \mu(\Omega_1 \cap \Omega_2)$.*

We may define a measure by selecting a $\psi \in \mathcal{H}$ and then defining the measure to be $\mu_\psi(\Omega) = \langle \psi, \mu(\Omega)\psi\rangle = ||\mu(\Omega)\psi||^2$. Observe that $\mu_\psi(\mathbb{R}) = ||\psi||^2 < \infty$. We may also construct a complex Borel measure via the polarization identity:

$$\mu_{\varphi,\psi}(\Omega) = \langle \varphi, \mu(\Omega)\psi\rangle = \frac{1}{4}(\mu_{\varphi+\psi}(\Omega) - \mu_{\varphi-\psi}(\Omega) + i\mu_{\varphi-i\psi}(\Omega) - i\mu_{\varphi+i\psi}(\Omega)).$$

Observe that, by Cauchy-Schwarz, $|\mu_{\varphi,\psi}| \leq ||\varphi|| \cdot ||\psi||$.

**Technicality** (Polarization identity): Let $A : \mathcal{D}_A \longrightarrow \mathcal{H}$ be a linear operator $q_A(\psi) = \langle \psi, A\psi \rangle$. Then the identity is:

$$\langle \varphi, A\psi \rangle = \frac{1}{4}(q_A(\varphi + \psi) - q_A(\varphi - \psi) + iq_A(\varphi - i\psi) - iq_A(\varphi + i\psi)).$$

Now, let us integrate with respect to a projection-valued measure. For every simple function,

$$f = \sum_{j=1}^{n} \alpha_j \chi_{\Omega_j},$$

where $\Omega_j = f^{-1}(\alpha_j)$, we define $\mathcal{P}(f)$ as,

$$\mathcal{P}(f) := \int_{\mathcal{B}} f \, d\mu = \sum_{j=1}^{n} \alpha_j \mu(\Omega_j).$$

Observe carefully that the above integral yields a sum of orthogonal projections, thus $\mathcal{P}(f)$ is not a number but rather an operator: $\mathcal{P}(f) \in \mathcal{L}(\mathcal{H})$. Indeed, observe that $\mathcal{P}(\chi_\Omega) = \mu(\Omega)$. By linearity of the integral, the operator $\mathcal{P}$ is a linear map from the set of simple functions into $\mathcal{L}(\mathcal{H})$.

Then from this, we may determine $\langle \varphi, \mathcal{P}(f)\psi \rangle$,

$$\begin{aligned} \langle \varphi, \mathcal{P}(f)\psi \rangle &= \sum_{j=1}^{n} \alpha_j \langle \varphi, \mu(\Omega_j)\psi \rangle \\ &= \sum_{j=1}^{n} \alpha_j \mu_{\varphi,\psi}(\Omega_j) \\ &= \int_{\mathbb{R}} f \, d\mu_{\varphi,\psi} \end{aligned} \tag{8}$$

and also,

$$\begin{aligned} ||\mathcal{P}(f)\psi||^2 &= \langle \sum_{j=1}^{n} \alpha_j \mu(\Omega_j)\psi, \sum_{i=1}^{n} \alpha_i \mu(\Omega_i)\psi \rangle \\ &= \sum_{j=1}^{n} |\alpha_j|^2 \cdot ||\mu(\Omega_j)\psi||^2 \\ &= \sum_{j=1}^{n} |\alpha_j|^2 \mu_\psi(\Omega_j) \\ &= \int_{\mathbb{R}} |f|^2 \, d\mu_\psi, \end{aligned} \tag{9}$$

where in the second line we used the fact that the sets $\Omega_j$ are disjoint.

If we equip the simple functions with the sup norm, we get $||\mathcal{P}(f)\psi|| \leq ||f||_\infty ||\psi||$ and hence, $\mathcal{P}$ has norm one. Since the simple functions are dense in $B(\mathbb{R})$ (the Banach space of bounded, complex-valued, measurable functions defined on $\mathcal{B}$), $\mathcal{P}$ can be extended to a unique bounded linear operator $\mathcal{P} : B(\mathbb{R}) \longrightarrow \mathcal{L}(\mathcal{H})$, where $\mathcal{P}$ still has norm one and (8) and (9) remain true.

**Theorem 1.** *Let $\mu$ be a projection-valued measure. Then the linear map,*

$$\mathcal{P} : B(\mathbb{R}) \longrightarrow \mathcal{L}(\mathcal{H})$$
$$f \longmapsto \int_{\mathcal{B}} f \, d\mu,$$

*is unique and satisfies the following properties:*

*(i)* $\langle \psi, \mathcal{P}(f)\psi \rangle = \int_{\mathbb{R}} f \, d\mu_\psi$ *for all* $f$ *and for all* $\psi \in \mathcal{H}$.

*(ii)* $\int_{\mathbb{R}} \chi_\Omega \, d\mu = \mu(\Omega)$, *for all* $\Omega \in \mathcal{B}$. *The integral of the constant function* $1$ *is* $\mathbb{I}$.

*(iii) For all* $f$, *we have* $|| \int_{\mathbb{R}} f \, d\mu|| \leq \sup_{\lambda \in \mathbb{R}} |f(\lambda)|$

*(iv) Multiplicativity: For all* $f$ *and* $g$, $\int_{\mathbb{R}} fg \, d\mu = (\int_{\mathbb{R}} f \, d\mu)(\int_{\mathbb{R}} g \, d\mu)$

*(v) For all* $f$, $\int_{\mathbb{R}} f^* \, d\mu = (\int_{\mathbb{R}} f \, d\mu)^*$

Now, for a densely defined, closed operator $A$, the resolvent set of $A$ is defined by,

$$\rho(A) = \{ \lambda \in \mathbb{C} \,|\, (A - \lambda)^{-1} \in \mathcal{L}(\mathcal{H}) \}.$$

That is, $\lambda \in \rho(A)$ if and only if $(A - \lambda) : \mathcal{D}_A \longrightarrow \mathcal{H}$ is bijective and its inverse is bounded.

The spectrum is defined by the complement of the resolvent set:

$$\sigma(A) = \mathbb{C} \setminus \rho(A).$$

That is, $\lambda \in \sigma(A)$ if $A - \lambda$ has a nontrivial kernel. Then a nonzero $\psi \in \mathrm{Ker}(A - \lambda)$ is called an eigenvector and $\lambda$ is called an eigenvalue.

**Theorem 2.** *If* $A$ *is a self-adjoint operator (bounded or unbounded), then* $\sigma(A)$ *is contained in the real line.*

We may now state the spectral theorem for bounded, self-adjoint operators.

**Theorem 3.** *If* $A \in \mathcal{L}(\mathcal{H})$ *is self-adjoint, then there exists a unique projection-valued measure* $\mu^A$ *on the Borel sigma algebra in* $\sigma(A)$, *with values in projections on* $\mathcal{H}$, *such that,*

$$\int_{\sigma(A)} \lambda \, d\mu^A(\lambda) = A \tag{10}$$

Using this spectral theorem, we may now define a functional calculus for bounded, self-adjoint operators.

**Definition.** *If* $A \in \mathcal{L}(\mathcal{H})$ *is self-adjoint and* $f : \sigma(A) \longrightarrow \mathbb{C}$ *is a bounded measurable function, we define the operator* $f(A)$ *as,*

$$f(A) := \int_{\sigma(A)} f(\lambda) \, d\mu^A(\lambda), \tag{11}$$

*where* $\mu^A$ *is the unique projection-valued measure associated to* $A$, *as mentioned in Theorem 3.*

**Remark.** *The projection-valued measure $\mu^A$ may be extended from $\sigma(A)$ to all of $\mathbb{R}$ by assigning measure zero to $\mathbb{R} \setminus \sigma(A)$.*

Now consider unbounded measurable functions on $\mathbb{R}$. Recall that earlier, we obtained,

$$||\mathcal{P}(f)\psi||^2 = \int_{\mathbb{R}} |f|^2 \, d\mu_\psi.$$

Then it seems reasonable that for unbounded $f$, we should define the domain,

$$\mathcal{D}_f = \{\, \psi \in \mathcal{H} \mid \int_{\mathbb{R}} |f(\lambda)|^2 \, d\mu_\psi(\lambda) < \infty \,\}. \tag{12}$$

We then get the following theorem.

**Theorem 4.** *Suppose $\mu : \mathcal{B} \longrightarrow \mathcal{L}(\mathcal{H})$ is a projection-valued measure and $f : \mathbb{R} \longrightarrow \mathbb{C}$ is a measurable, possibly unbounded, function. Then the operator*

$$\mathcal{P}(f) := \int_{\mathbb{R}} f \, d\mu$$

*whose domain is $\mathcal{D}_f$, is unbounded, unique, and satisfies the following properties:*

*(i) For all $\psi \in \mathcal{D}_f$, we have $\langle \psi, \mathcal{P}(f)\psi \rangle = \int_{\mathbb{R}} f(\lambda) \, d\mu_\psi(\lambda)$*

*(ii) For all $\psi \in \mathcal{D}_f$, we have $||\mathcal{P}(f)\psi||^2 = \int_{\mathbb{R}} |f|^2 \, d\mu_\psi$*

**Remark.** *If $f$ is bounded, then the domain of $\mathcal{P}(f)$ is all of $\mathcal{H}$, so that in this particular case, the integral $\mathcal{P}(f)$ in Theorem 4 agrees with the integral in Theorem 1. Thus, if $f$ is a bounded function, then $\mathcal{P}(f)$ will be a bounded operator.*

We may now state the spectral theorem for a general self-adjoint operator.

**Theorem 5.** *Suppose $A$ is a self-adjoint operator on $\mathcal{H}$. Then there is a unique projection-valued measure $\mu^A$ on $\sigma(A)$ with values in $\mathcal{L}(\mathcal{H})$ such that,*

$$\int_{\sigma(A)} \lambda \, d\mu^A(\lambda) = A. \tag{13}$$

Just as we did earlier, we use the spectral theorem to define a functional calculus for general self-adjoint operators.

**Definition.** *For any measurable function $f$ on $\sigma(A)$, we define the operator $f(A)$, which is possibly unbounded, by,*

$$f(A) = \int_{\sigma(A)} f(\lambda) \, d\mu^A(\lambda). \tag{14}$$

As before, we can extend the projection-valued measure $\mu^A$ from $\sigma(A)$ to all of $\mathbb{R}$.

## Time Evolution of the Schrödinger Equation

Consider the following initial value problem of the Schrödinger equation,

$$-i\frac{d}{dt}\psi(t) = H\psi(t), \qquad \psi(0) = \psi_0 \in \mathcal{D}_H, \tag{15}$$

where $H$ is the Hamiltonian (the operator corresponding to the energy of the system). Recall that $\psi(t) = U(t)\psi_0$ and so with this, the above equation becomes,

$$-i\frac{d}{dt}U(t) = HU(t)$$

which then suggests that our unitary operators should have the form $U(t) = e^{itH}$. This would then mean that the solution to (15) is

$$\psi(t) = e^{itH}\psi_0. \tag{16}$$

For all of this to work, we must show that $U(t) = e^{itH}$ is in line with Axiom 4; that is, we must show that it defines a strongly continuous one-parameter unitary group whose generator corresponds to $H$.

**Theorem 6.** *Let $A$ be a self-adjoint operator on $\mathcal{H}$ and let $U(\cdot)$ be defined by $U(t) = e^{itA}$, $t \in \mathbb{R}$, where the operator $e^{itA}$ is defined by the functional calculus for $A$. Then:*

*(i)* *$U(t)$ is a strongly continuous one-parameter unitary group.*

*(ii)* *For all $\psi \in \mathcal{D}_A$,*

$$A\psi = \lim_{t\to 0}\frac{1}{i}\frac{U(t)\psi - \psi}{t}$$

*(iii)* *For all $\psi \in \mathcal{H}$, if the limit,*

$$\lim_{t\to 0}\frac{1}{i}\frac{U(t)\psi - \psi}{t}$$

*exists, then $\psi \in \mathcal{D}_A$ and the limit is equal to $A\psi$.*

*(iv)* *If $\psi \in \mathcal{D}_A$, then for all $t \in \mathbb{R}$, we have $U(t)\psi \in \mathcal{D}_A$ and,*

$$\lim_{h\to 0}\frac{U(t+h)\psi - U(t)\psi}{h} = iU(t)A\psi = iAU(t)\psi.$$

*Proof.* Define the function $f(\lambda) = e^{it\lambda}$. Since $\sigma(A) \subset \mathbb{R}$, $f(\lambda)$ is bounded on $\sigma(A)$ and satisfies $f(\lambda)f(\lambda)^* = 1$ for all $\lambda \in \sigma(A)$. Then $f(A)$ is bounded and has the properties listed in Theorem 1. Properties $(ii), (iv)$, and $(v)$ of Theorem 1 give $f(A)f(A)^* = f(A)^*f(A) = \mathbb{I}$ and hence, $f(A)$ is unitary. Then the multiplicativity of the functional calculus shows that $U(t)$ is indeed a one-parameter unitary group.

For strong continuity, consider,

$$||U(t)\psi - U(s)\psi||^2 = \int_{\mathbb{R}} |e^{it\lambda} - e^{is\lambda}|^2 \, d\mu_\psi^A(\lambda).$$

Taking $\lim_{s\to t}$ of the above, we can apply dominated convergence to the integral to see that it goes to zero and hence, we have strong continuity.

For the second part of the theorem, recall that, by the spectral theorem for unbounded operators, $A = \int_{\mathbb{R}} \lambda \, d\mu^A(\lambda)$. Consider $\psi \in \mathcal{D}_A$. Then,

$$||\frac{1}{i}\frac{U(t)\psi - \psi}{t} - A\psi||^2 = \int_{\mathbb{R}} |\frac{1}{i}\frac{e^{it\lambda} - 1}{t} - \lambda|^2 d\mu_\psi^A(\lambda) \tag{17}$$

Now, observe that,

$$\begin{aligned} e^{it\lambda} - 1 &= \int_0^\lambda ite^{ity} dy \\ \Rightarrow |e^{it\lambda} - 1| \leq |t| &\int_0^\lambda |e^{it\lambda}| dy \leq |t\lambda|. \end{aligned}$$

Also, note that $\psi \in \mathcal{D}_A$, with $A = \int_{\mathbb{R}} \lambda \, d\mu^A(\lambda)$, gives $\int_{\mathbb{R}} \lambda^2 \, d\mu_\psi^A(\lambda) < \infty$. Combining these facts allows us to apply dominated convergence to (17) (by using $4\lambda^2$ as the dominating function). Expressing the integrand in (17) as a Taylor expansion, it is easy to see that its limit will tend to zero, hence the entire integral will tend to zero, hence we have the second part of the theorem.

For the third part of the theorem, suppose $\tilde{A}$ is the infinitesimal generator of $U(\cdot)$. If $\psi, \phi \in \mathcal{D}_{\tilde{A}}$, then,

$$\begin{aligned} \langle \phi, \tilde{A}\psi \rangle &= \lim_{t\to 0} \langle \phi, \frac{1}{i}\frac{U(t)\psi - \psi}{t} \rangle \\ &= \lim_{t\to 0} \langle -\frac{1}{i}\frac{U(t)^*\phi - \phi}{t}, \psi \rangle \\ &= \lim_{t\to 0} \langle \frac{1}{i}\frac{U(-t)\phi - \phi}{(-t)}, \psi \rangle \\ &= \langle \tilde{A}\phi, \psi \rangle \, . \end{aligned}$$

This calculation shows that $\tilde{A}$ is symmetric. Additionally, note that if $\psi, \phi \in \mathcal{D}_A$, then the second part of the theorem says that the infinitesimal generator is $A$, so that our $\tilde{A}$ is an extension of $A$. Then, by the fact (which is not proven here) that self-adjoint operators are maximal, meaning they have no symmetric extensions, we must have $\tilde{A} = A$.

For the fourth part of the theorem, observe that,

$$\frac{U(t+h)\psi - U(t)\psi}{h} = U(t)\frac{U(h)\psi - \psi}{h},$$

so that if $\psi \in \mathcal{D}_A$ and if we take $\lim_{h\to 0}$ of the above, then the right hand side becomes $iU(t)A\psi$.

At the same time, we have,

$$\frac{U(t+h)\psi - U(t)\psi}{h} = \frac{U(h)(U(t)\psi) - (U(t)\psi)}{h},$$

so that if we now take $\lim_{h\to 0}$ of the above, we get, by definition, $iA(U(t)\psi)$. Thus, $U(t)\psi \in \mathcal{D}_A$.

□

So, given the Hamiltonian operator $H$, which corresponds to the energy of the system, we know that it is self-adjoint (by the previous section). Then by the above theorem, $H$ is the infinitesimal generator for the strongly continuous one-parameter unitary group $U(\cdot)$ defined by $U(t) = e^{itH}$. Then with the fourth point in the above theorem, we can now say that $\psi(t) = e^{itH}\psi_0$ is indeed the solution to the Schrödinger equation, provided that $\psi_0 \in \mathcal{D}_H$.

# References

[1] B. C. Hall. *Quantum Theory for Mathematicians*, Graduate Texts in Mathematics, 267, Springer, 2013.

[2] G. Teschl. *Mathematical Methods in Quantum Mechanics: With Applications to Schrödinger Operators*, 2nd Edition, Graduate Studies in Mathematics, Vol. 157, American Mathematical Society, 2014.