EE Group 5

Mathematics

RQ:

How does abstract mathematics apply to physical phenomena in the process of the development of Schrodinger's equations?

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1 Introduction

Mathematics is a field of research acclaimed for elegance and functionality, but often criticised for its abstract nature. In the educational environment, this becomes evident with the arbitrary introduction of concepts such as vector spaces and complex numbers, with no immediate grounding in physical reality. This essay approaches the issue with an aim to uncover the applications of mathematics and the reasoning behind selecting abstract concepts with consideration of their use in elementary quantum mechanics (QM). Arguably, elementary QM lies in Erwin Schrodinger's work on the time-dependent Schrodinger equation (TDSE) and time-independent Schrodinger equation (TISE). This led to the research question: **How does abstract mathematics apply to physical phenomena in the process of the development of Schrodinger's equations?** QM is used as context for the discussion of mathematics' application to the natural sciences, providing justification for continued mathematical research as a means of supporting science.

The scope of this essay is dictated by Barton Zweibach's lectures in Quantum Physics at MIT. Mathematics outside these lectures is considered, but remains at a freshman undergraduate level. The essay uses secondary sources which review research articles from prominent physicists and mathematicians who contributed to the foundation of QM such as Dirac, Schrodinger, von Neumann and Hilbert. A strong focus is maintained on linear algebra and differential calculus.

2 Physics

2.1 Wave-function

Probability is the foundation of QM. For a given free particle (a particle not bounded by external forces), the probability is modelled by an amplitude function, commonly written as $\Psi(x,t)$. It is a wave-function that changes with respect to position, x, and time, t. Note that x is usually a position vector, $\vec{x}$, but for simplicity, extra spatial dimensions are avoided. $\Psi(x,t)$ outputs a complex number, which lies on the complex plane (or space). The complex number's magnitude (or norm) is the value of the amplitude outputted by the function [Zwe16a].

Similar to classical physics, where the intensity of an electromagnetic wave is proportional to amplitude, the probability of a free particle appearing at (x,t) in space-time, is given by $|\Psi(x,t)|^2$ (amplitude squared) [Sch16]. Note that $|\Psi(x,t)|^2 = \Psi(x,t)^*\Psi(x,t)$, since Ψ is a complex-valued function. The particle must always exist in space, so the total probability over all space must equal to 1:

$$\int_{-\infty}^{\infty} |\Psi(x,t)|^2 \partial x = \int_{-\infty}^{\infty} \Psi(x,t)^* \Psi(x,t) \partial x = 1 \tag{2.1}$$

This is important to note for Section 4.8.

2.2 Phase Shift

Since the free particle is modelled by a wave-function, it seems natural to define the particle with respect to its wave properties. One such important property is a phase, which is an angle manipulated with respect to time and position to output an amplitude. To aid with future derivations, both the momentum and energy must be considered in the phase.

For this, the de-Broglie wavelength, λ, is used [Zwe16c].

$$p = \frac{h}{\lambda} \tag{2.2}$$

λ provides a connection between the momentum of a particle (p) and wavelength of the wave-function. One might postulate that λ itself can be used as a phase, since it happens to change as x changes. However, since the phase refers to an angular quantity, it is important to represent momentum with reference to an angular quantity, which λ is not. Hence:

$$p = \frac{h}{\lambda} = \frac{h}{2\pi}\frac{2\pi}{\lambda} = \hbar k \tag{2.3}$$

$\hbar$ is called the reduced Planck constant. k is known as the "angular wavenumber". $\frac{1}{\lambda}$ represents how many times per unit distance the wavelength appears. $k = \frac{2\pi}{\lambda}$ represents how many radians the wave-function sweeps through on the unit circle per unit distance. Since k is angular, it can be incorporated easily into the phase.

Similarly, the Planck-Einstein relation can use the energy of a particle to find an angular quantity. This is [Zwe16c]:

$$E = hf \tag{2.4}$$

and to model frequency as an angular quantity:

$$E = hf = \frac{h}{2\pi}2\pi f = \hbar\omega \tag{2.5}$$

ω is the angular frequency of the wave. These give the de-Broglie relations:

$$p = \hbar k \text{ and } E = \hbar\omega \tag{2.6}$$

It is important to notice that ω is actually a function of k.

$$k = \frac{2\pi}{\lambda} = \frac{2\pi f}{v} = \frac{\omega}{v} \implies \omega(k) = kv \tag{2.7}$$

Hence, two angular quantities have been determined. k can be evolved with respect to position, such that kx is a certain phase shift. Similarly, ω, can be evolved with respect to time, such that ωt is a certain phase shift. Combining the two, an overall phase shift is $\Phi = kx - \omega t$.

2.3 The Ansatz:

As for the wave-function's general mathematical form, a "guess" must be made. QM, and many fields of mathematics and physics, require such "guesses", since there might not be another way to approach the problem. Popularised by Leonhard Euler, it is known as an "ansatz". An educated, intelligent starting point.

Several possible wave-functions can be tested, provided the following conditions are satisfied.

- Output a periodic amplitude,
- Have total probability of 1 over space,
- Never be zero for all values of x at a given time (this would mean the particle simply disappeared),
- Satisfy the above conditions for any superposition (linear combination of wave-functions), discussed further in Section 4.3.

There are 4 possibilities of the wave-function which satisfy the above conditions [Zwe16c]:

1. $\Psi(x,t) = \sin(kx - \omega t)$
2. $\Psi(x,t) = \cos(kx - \omega t)$
3. $\Psi(x,t) = e^{i(kx - \omega t)}$
4. $\Psi(x,t) = e^{i(\omega t - kx)}$

The first three conditions are satisfied for all 4 functions, but the final condition must be tested for.

Testing for the Ansatz

1. $\boldsymbol{\Psi(x,t) = \sin(kx - \omega t)}$:

Consider the wave-function $\Theta(x,t) = \Psi(x,t) + \Psi(x,-t)$, such that $\Theta(x,t)$ represents the superposition of the wave-functions moving in the $+t$ direction and the $-t$ direction. These are perfect opposites of one another with respect to time. This superposition is chosen to conduct a proof by contradiction.

$$\begin{aligned}\Theta(x,t) &= \sin(kx - \omega t) + \sin(kx + \omega t) \\ &= \sin(kx)\cos(\omega t) - \cos(kx)\sin(\omega t) + \sin(kx)\cos(\omega t) + \cos(kx)\sin(\omega t) \\ &= 2\sin(kx)\cos(\omega t)\end{aligned}$$

This superposition poses a problem. Whenever $\omega t = \frac{\pi}{2}, \frac{3\pi}{2}, ...$, Θ has a value of 0. Hence, there exists t such that for all $x : \Theta(x,t) = 0$. The particle disappears, rendering the wave-function invalid.

2. $\boldsymbol{\Psi(x,t) = \cos(kx - \omega t)}$:

Again, consider $\Theta(x,t) = \Psi(x,t) + \Psi(x,-t)$.

$$\begin{aligned}\Theta(x,t) &= \cos(kx-\omega t) + \cos(kx+\omega t)\\ &= cos(kx)\cos(\omega t) + \sin(kx)\sin(\omega t) + \cos(kx)\cos(\omega t) - \sin(kx)\sin(\omega t)\\ &= 2\cos(kx)\cos(\omega t)\end{aligned}$$

Similarly, whenever $\omega t = \frac{\pi}{2}, \frac{3\pi}{2}, ...$ Θ has a value of 0. Hence there exists t such that for all $x : \Theta(x,t) = 0$. Again, the wave-function is invalid.

3. $\boldsymbol{\Psi(x,t) = e^{i(kx-\omega t)}}$:

Consider $\Theta(x,t) = \Psi(x,t) + \Psi(-x,t)$, which is a superposition of wave-functions with opposite values with respect to position. Again, this is an arbitrary selection.

$$\begin{aligned}\Theta(x,t) &= e^{i(kx-\omega t)} + e^{i(-kx-\omega t)}\\ &= \left(e^{ikx} + e^{-ikx}\right)e^{-i\omega t}\\ &= (\cos(kx) + i\sin(kx) + \cos(kx) - i\sin(kx))e^{-i\omega t}\\ &= 2\cos(kx)e^{-i\omega t}\end{aligned}$$

Under this superposition, for all $x, t : \Theta(x,t) \neq 0$. This is because for all $t : e^{-i\omega t} \neq 0$. Similarly, 4. also works. However, in physics, it is convention to use 3. Hence, the free particle wave-function can be modelled as [Zwe16c]:

$$\Psi(x,t) = e^{ikx-i\omega t} \tag{2.8}$$

Unfortunately, this definition is simplified and models a singular "plane wave".

However, not all particles are plane waves with a unique wavenumber, k. Most particles are a combination of these singular wavenumber plane waves. The most generalised form of the free particle wave-function involves a superposition of every possible plane wave [Zwe16d].

$$\Psi(x,t) = \int_{-\infty}^{\infty} \Phi(k) e^{ikx - i\omega t} \mathrm{d}k \tag{2.9}$$

This integral is the Fourier series combination of every possible sinusoidal function. $\Phi(k)$ is a coefficient function which controls the weighting of each wave-function in the superposition. This is the true free-particle wave-function. For the course of this essay, the simplified variation will be used, but any results for the simplified variation will apply to the free-particle.

Interestingly, complex numbers have nestled their way into the wave-function. Schrodinger hadn't yet comprehended the appearance of complex numbers, writing in a letter to Hendrik Lorentz that "Ψ is surely fundamentally a real function" [Sch26]. This bewilderment is understandable, considering the function should describe the real world. It just happened to be that complex numbers were the conventional method of creating a vector valued function at the time. Feynman went on to describe a wave-function like a dial going around a circle in QED, breaking the myth that complex numbers were crucial [Fey85].

This probes the necessity of an abstract mathematical structure like the complex plane [Kar19]. However, to a practical physicist, the necessity of a structure doesn't impact its effectiveness. Schrodinger continued to use complex numbers, even if it seemed impossible [Sch26].

3 Operators

An operator is an object which scales a vector by a constant [Sim09]. The wave-function acts as a vector in this context.

3.1 The Momentum Operator

The purpose of the momentum operator is to operate upon Ψ to extract information regarding the momentum.

$$\begin{aligned}\frac{\hbar}{i}\frac{\partial}{\partial x}\Psi(x,t) &= \frac{\hbar}{i}\frac{\partial}{\partial x}e^{ikx-i\omega t}\\ &= \frac{\hbar}{i}(ik)e^{ikx-i\omega t}\\ &= (\hbar k)e^{ikx-i\omega t}\\ &= pe^{ikx-i\omega t}\end{aligned}$$

$$\frac{\hbar}{i}\frac{\partial}{\partial x}\Psi(x,t) = p\Psi(x,t) \tag{3.1}$$

Applying $\frac{\hbar}{i}\frac{\partial}{\partial x}$ upon the wave-function scales it by the momentum. The operation is known as the momentum operator, $\hat{p}$ [Zwe16b].

$$\hat{p} = \frac{\hbar}{i}\frac{\partial}{\partial x} \tag{3.2}$$

$$\hat{p}\Psi(x,t) = p\Psi(x,t) \tag{3.3}$$

3.2 The Energy Operator

The momentum operator differentiated with respect to position to extract k, which is associated with momentum. The energy operator can differentiate with respect to time, extracting ω which is associated with energy.

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = i\hbar(-i\omega)\Psi(x,t) = E\Psi(x,t) \tag{3.4}$$

While differentiating with respect to time is useful, it doesn't allow for a connection to the momentum operator (essential to derive Schrodinger's equations). The momentum-energy relation can fix this.

$$E = \frac{1}{2}mv^2 = \frac{1}{2}\frac{(mv)^2}{m} = \frac{p^2}{2m} \tag{3.5}$$

The relation can be used to construct the energy operator by replacing p with the momentum operator [Zwe16b].

$$\begin{aligned}
&E\Psi(x,t)\\
&= \frac{p^2}{2m}\Psi(x,t)\\
&= \frac{p}{2m}p\Psi(x,t)\\
&= \frac{p}{2m}\frac{\hbar}{i}\frac{\partial}{\partial x}\Psi(x,t)\\
&= \frac{1}{2m}\frac{\hbar}{i}\frac{\partial}{\partial x}\frac{\hbar}{i}\frac{\partial}{\partial x}\Psi(x,t)\\
&= -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t)
\end{aligned}$$

This defines the energy operator:

$$\hat{E} = \frac{\hat{p}}{2m} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} \tag{3.6}$$

Noting this result, one can put together Eq. 3.4 and Eq. 3.6 to create the Schrodinger equation [Zwe16b].

$$-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\Psi(x,t) = i\hbar\frac{\partial}{\partial t}\Psi(x,t) \tag{3.7}$$

4 The Linear Algebra

4.1 TISE

The energy operator is usually replaced by the Hamiltonian operator, $\hat{H}$. The Hamiltonian is associated with finding the total energy in the system, including potential energy (which was ignored, for simplicity) [Nav16]. Since the Hamiltonian is applied on the wave-function in a vector space, it can be characterised as a matrix.

$$\hat{H}\Psi(x,t) = i\hbar\frac{\partial}{\partial t}\Psi(x,t) \tag{4.1}$$

This equation is the TDSE, since it models change with respect to time of a wave-function. However, the energy operator, $\hat{E} = i\hbar\frac{\partial}{\partial t}$, can be replaced with E, since the effect of the Hamiltonian operator is to find total energy. This inadvertently eliminates any time dependent components from the equation, providing the TISE [BH20]:

$$\hat{H}\Psi(x) = E\Psi(x) \tag{4.2}$$

Both equations apply differently to the real world. The TISE can model states of particles which do not change with respect to time: energy levels of an electron on a hydrogen atom [HH20]. The TDSE can model states that change with respect to time: modelling an electron's movement in a changing electric field.

4.2 Eigenvalue Equation

The Schrodinger's equations happen to have connections to linear algebra concepts. A matrix is a set of values which describes a linear transformation [Bee17]. An important property of a linear transformation are eigenvectors. These vectors satisfy:

$$M\vec{v} = a\vec{v} \tag{4.3}$$

The transformation scales the eigenvectors by a constant, a, known as the eigenvalue. [Wei20a]. The TISE (Eq. 4.2) is a characteristic eigenvalue equation. $\hat{H}$ is the matrix, E is an eigenvalue of $\hat{H}$, and Ψ is the eigenvector, otherwise referred to as the eigenstate. The solutions to the TISE are eigenstates, and the corresponding eigenvalues represent total energy values. Similarly, in Eq. 3.3, $\hat{p}$ is an operator which solves for the momentum eigenvalue.

4.3 Linearity

The Hamiltonian satisfies the superposition principle, enough to show that it is a linear operator [Zwe16a]:

$$\begin{aligned} &\text{If } \hat{L}\vec{v} = 0, \\ &\textbf{Additivity:} && \hat{L}(\vec{v}_1 + \vec{v}_2) = \hat{L}\vec{v}_1 + \hat{L}\vec{v}_2 \\ &\textbf{Homogeneity:} && \hat{L}(\alpha\vec{v}) = \alpha\hat{L}\vec{v} \\ &\textbf{Superposition Principle:} && \hat{L}(\alpha\vec{v}_1 + \beta\vec{v}_2) = \alpha\hat{L}\vec{v}_1 + \beta\hat{L}\vec{v}_2 \end{aligned} \tag{4.4}$$

The conditions of additivity and homogeneity give the superposition principle [Hee]. In physics, a system described by a linear operator is generally easiest to work with. The Navier-stokes equations on fluid mechanics are notorious partly due to their non-linear nature. However, QM is generally linear. Eq. 4.1 can be rewritten to show the superposition principle,

$$\begin{aligned} \hat{H}\Psi(x,t) - i\hbar\frac{\partial}{\partial t}\Psi(x,t) &= 0 \\ \left(\hat{H} - i\hbar\frac{\partial}{\partial t}\right)\Psi(x,t) &= 0 \\ \hat{L}\Psi(x,t) &= 0 \end{aligned}$$

An application of $\hat{H}$, multiplication by $i\hbar$, and differentiation with respect to time, are all linear operations. Hence, the entire operator is linear. This makes Schrodinger's equations an appealing model for QM with the added benefit of being able to linearly combine wave-functions [Dir58].

4.4 The Eigenstates

Any wave-function of a particle can be represented as a superposition of much simpler wave-functions. The generalised free particle wave-function (Eq. 2.9) represents it mathematically with a Fourier series composed of "simple" wave-functions. These "simple" wave-functions are eigenstates, solutions to the TISE. Using linear combinations of eigenstates, any wave-function can be represented.

This is similar to representing vectors as linear combinations of their unit vectors:

$$\begin{bmatrix} a \\ b \\ c \end{bmatrix} = a\begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix} + b\begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix} + c\begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix}$$

Similarly in QM:

$$\Psi = \sum_{n=1} b_n \varphi_n \tag{4.5}$$

where each b_n is a coefficient for each eigenstate, φ_n [Dwo]. The eigenstates behave like unit vectors, which span their vector space of $\mathbb{R}^3$. The conditions of a vector space are the preservation of vector addition and scalar multiplication [Qui+14]. The TDSE has been shown to support this with the superposition principle.

In a physical context, eigenstates are the possible states of the system [Dir58]. The Fourier sum takes into account the "weightage" or probability of each possible state with the $\Phi(k)$ function as a coefficient (further explored in Section 4.8). More importantly, each eigenstate has a corresponding eigenvalue in the TISE. The eigenvalues are measurable properties in the physical world, and with the TISE, the eigenvalue represents total energy values. In real life, when a certain eigenvalue (or energy) is measured, it corresponds to it's eigenstate. Then, the particle collapses to the eigenstate [Alf08]. This is popularly referred to as "collapsing the wave-function".

4.5 Hermitian Matrix

While the eigenstates can span a vector space, they also have other interesting properties with reference to the TISE:

1. The measured eigenvalues of the TISE are always real since they represent physical properties (the TISE, specifically, models totals energy) [Wei20b].
2. The eigenvectors of the Hamiltonian matrix are orthonormal [Wei20b]. This means there are n distinct eigenstates spanning an n-dimensional space and they are all perpendicular to one another.

These conditions exist because the Hamiltonian operator is Hermitian. This is a special characteristic where the complex conjugate transpose of a matrix is equal to itself:

$$(A^*)^T = A^\dagger = A \tag{4.6}$$

4.6 Proof of Hermiticity

The formal condition of hermiticity for $\hat{H}$ is [Gri04]:

$$\int_{-\infty}^{\infty} \Psi^* \hat{H} \Psi \partial x = \int_{-\infty}^{\infty} (\hat{H}\Psi)^* \Psi \partial x \tag{4.7}$$

This formality can be intuitively confirmed. The probability of a wave-function over all space is:

$$\int_{-\infty}^{\infty} |\Psi|^2 \partial x = \int_{-\infty}^{\infty} \Psi^* \Psi \partial x = 1 \tag{4.8}$$

Applying a transformation to the initial state of the wave-function ($(\hat{H}\Psi)^*$) or the final state of the wave-function ($\hat{H}\Psi$) will always result in a probability of 1 [Gri04]. Nevertheless, this result isn't at all mathematically obvious. The Hamiltonian operator ($\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} = i\hbar\frac{\partial}{\partial t}$) can be shown to satisfy this condition:

$$\int_{-\infty}^{\infty} \Psi^* i\hbar \frac{\partial \Psi}{\partial t} \partial x$$

This can be solved with integration by parts:

$$u = \Psi^* i\hbar \qquad v = \int \frac{\partial \Psi}{\partial t} \partial x$$

$$\partial u = \frac{\partial \Psi^*}{\partial x} i\hbar \partial x \qquad \partial v = \frac{\partial \Psi}{\partial t} \partial x$$

$$\begin{aligned}
\int_{-\infty}^{\infty} \Psi^* i\hbar \frac{\partial \Psi}{\partial t} \partial x &= \left(\Psi^* i\hbar \int \frac{\partial \Psi}{\partial t} \partial x\right)\Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \int \frac{\partial \Psi}{\partial t} \partial x \frac{\partial \Psi^*}{\partial x} i\hbar \partial x \\
&= \left(\Psi^* \int i\hbar \frac{\partial \Psi}{\partial t} \partial x\right)\Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \int i\hbar \frac{\partial \Psi}{\partial t} \partial \Psi^* \partial x \\
&= \left(\Psi^* \int \hat{H}\Psi \partial x\right)\Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} \int i\hbar \frac{\partial \Psi}{\partial t} \partial \Psi^* \partial x
\end{aligned}$$

Ψ and Ψ^* both evaluate to 0 at positive and negative infinity, which is characteristic of a free-particle whose probability falls to 0 at extremes.

$$\begin{aligned}
\int_{-\infty}^{\infty} \Psi^* i\hbar \frac{\partial \Psi}{\partial t} \partial x &= -\int_{-\infty}^{\infty} \int i\hbar \frac{\partial \Psi}{\partial t} \partial \Psi^* \partial x \\
&= -\int_{-\infty}^{\infty} i\hbar \frac{\partial \Psi^*}{\partial t} \Psi \partial x \\
&= -\int_{-\infty}^{\infty} -(i\hbar)^* \left(\frac{\partial \Psi}{\partial t}\right)^* \Psi \partial x \\
&= \int_{-\infty}^{\infty} \left(i\hbar \frac{\partial \Psi}{\partial t}\right)^* \Psi \partial x \\
&= \int_{-\infty}^{\infty} (\hat{H}\Psi)^* \Psi \partial x \\
\int_{-\infty}^{\infty} \Psi^* \hat{H} \Psi \partial x &= \int_{-\infty}^{\infty} (\hat{H}\Psi)^* \Psi \partial x
\end{aligned}$$

The Hamiltonian operator is hermitian. In fact, any observable operator (such as the momentum operator) will demonstrate hermiticity [Gri04].

4.7 Proof of Properties of Hermiticity

To show that the eigenvalues of the matrix are real:

$$A\vec{v} = \lambda\vec{v}$$

$$(A\vec{v})^\dagger = (\lambda\vec{v})^\dagger$$

$$\vec{v}^\dagger A^\dagger = \lambda^\dagger \vec{v}^\dagger$$

$$\vec{v}^\dagger A^\dagger \vec{v} = \lambda^\dagger \vec{v}^\dagger \vec{v}$$

$$\vec{v}^\dagger A \vec{v} = \lambda^\dagger \vec{v}^\dagger \vec{v}$$

$$\vec{v}^\dagger \lambda \vec{v} = \lambda^\dagger \vec{v}^\dagger \vec{v}$$

$$\lambda \vec{v}^\dagger \vec{v} = \lambda^\dagger \vec{v}^\dagger \vec{v}$$

$$\lambda = \lambda^\dagger$$

Hence λ must be real [Qua12]. Secondly, to show that the eigenvectors are orthonormal. Let there be n distinct eigenvalues for the $n \times n$ matrix, A, and let λ_1, λ_2 be two of these eigenvalues.

$$A\vec{x} = \lambda_1 \vec{x}$$

$$A\vec{y} = \lambda_2 \vec{y}$$

Consider $\vec{x} \cdot A\vec{y}$:

$$= \vec{x} \cdot A\vec{y}$$

$$= (A\vec{y})^\dagger \vec{x}$$

$$= \vec{y}^\dagger A^\dagger \vec{x}$$

$$= \vec{y}^\dagger A \vec{x}$$

$$= \vec{y}^\dagger \lambda_1 \vec{x}$$

$$= \lambda_1 \vec{y}^\dagger \vec{x}$$

$$= \lambda_1 \vec{x} \cdot \vec{y}$$

Alternatively:

$$= \vec{x} \cdot A\vec{y}$$

$$= \vec{x} \cdot \lambda_2 \vec{y}$$

$$= \lambda_2 \vec{x} \cdot \vec{y}$$

Hence,

$$\lambda_1 \vec{x} \cdot \vec{y} = \lambda_2 \vec{x} \cdot \vec{y}$$

If $\vec{x} \cdot \vec{y} \neq 0$, then $\lambda_1 = \lambda_2$, which contradicts λ_1, λ_2 being distinct. Hence, $\vec{x} \cdot \vec{y} = 0$, and are orthonormal. All eigenvectors of A are orthonormal [Qua16].

Hermiticity is necessity for a wave-function to be decomposed into orthonormal eigenstates, because they are required to form a basis for the space which wave-functions exist in. This vector space can be thought of as an ∞-dimensional Euclidean space ($\mathbb{R}_\infty$), spanned by eigenstates.

David Hilbert first formalised an ∞-dimensional Euclidean space, which was later called a Hilbert space and applied to QM by John von Neumann [Neu55]. The Hilbert space isn't just a vector space, but it is a vector space where all vector functions are square-integrable ($\int_{-\infty}^{\infty} |\Psi|^2 \partial x = 1$) [Gri04]. This is consistent with knowledge about probability. Mathematically, this means that each eigenstate, and its linear combinations, are normalised [Sch16], always having a total probability equal to 1.

The Hilbert space speaks towards the role of mathematics in physics. Some mathematicians argue that mathematics describes the simplest concepts, hence any physical formalism will inevitably use mathematics. But this position assumes that the mathematics behind the formalism is actually simple. The Hilbert space is not a simple or obvious application [Wig60]. It is especially chosen for its unique properties, not by coincidence. It allows for a decomposition of the wave-function into eigenstates, allows for strictly real eigenvalues and allows for strictly normalised wave-functions. Using these properties of mathematics in physics leads to remarkable results, because even though mathematics is an incredibly abstract language, it is an incredibly accurate and effective language [Wig60].

4.8 Probability

This information allows for deeper analysis of the coefficients in the superpositions of wave-functions. It is important that:

$$\int_{-\infty}^{\infty} |\Psi(x,t)|^2 \partial x = 1 \tag{4.9}$$

Consider the wave-function $\Psi(x,t)$ represented as shown in Equation 4.5:

$$\Psi(x,t) = \sum_{n=1} b_n \varphi_n = b_1\varphi_1(x,t) + b_2\varphi_2(x,t) + \cdots + b_n\varphi_n(x,t)$$

In this case, the probability of each eigenstate and its coefficient must sum up to the probability of the original wave-function. This follows from the principle of superposition. The bounds from $-\infty$ to ∞ are ignored for clarity.

$$\begin{aligned}
\int |\Psi(x,t)|^2 \partial x &= \int |b_1\varphi_1(x,t)|^2 + |b_2\varphi_2(x,t)|^2 + \cdots + |b_n\varphi_n(x,t)|^2 \partial x && = 1 \\
&= \int |b_1|^2|\varphi_1(x,t)|^2 + |b_2|^2|\varphi_2(x,t)|^2 + \cdots + |b_n|^2|\varphi_n(x,t)|^2 \partial x && = 1 \\
&= \int |b_1|^2|\varphi_1(x,t)|^2 \partial x + \int |b_2|^2|\varphi_2(x,t)|^2 \partial x + \cdots + \int |b_n|^2|\varphi_n(x,t)|^2 \partial x && = 1 \\
&= |b_1|^2 \int |\varphi_1(x,t)|^2 \partial x + |b_2|^2 \int |\varphi_2(x,t)|^2 \partial x + \cdots + |b_n|^2 \int |\varphi_n(x,t)|^2 \partial x && = 1
\end{aligned}$$

Each $\int |\varphi_n(x,t)|^2 \partial x$ has a value of 1 since every $\varphi_n(x,t)$ is a normalised wave-function shown in Section 4.7 [Neu55]. Hence:

$$|b_1|^2 + |b_2|^2 + \cdots + |b_n|^2 = 1 \tag{4.10}$$

This is the relationship between the coefficients, relevant in Section 5.3.

5 The Equation

5.1 Time Evolution

Schrodinger's equation is a differential equation, and the TDSE is first order (only first derivative), allowing for it to be solved with separation of variables:

$$i\hbar\frac{\partial}{\partial t}\Psi(x,t) = \hat{H}\Psi(x,t)$$

$$\begin{aligned}
\frac{i\hbar}{\hat{H}}\frac{1}{\Psi(x,t)}\partial\Psi(x,t) &= \partial t \\
\frac{i\hbar}{\hat{H}}\int\frac{1}{\Psi(x,t)}\partial\Psi(x,t) &= \int\partial t \\
\frac{i\hbar}{\hat{H}}\ln\Psi(x,t) &= t + C \\
\ln\Psi(x,t) &= \frac{-i\hat{H}}{\hbar}t + C \\
\Psi(x,t) &= e^{\frac{-i\hat{H}}{\hbar}t+C} \\
\Psi(x,t) &= Ce^{\frac{-i\hat{H}}{\hbar}t}
\end{aligned}$$

Consider $\Psi(x,t)$ at $t = 0$:

$$\Psi(x,0) = Ce^{\frac{-i\hat{H}}{\hbar}(0)}$$

$$\Psi(x,0) = C$$

Hence time evolution is modelled by:

$$\Psi(x,t) = e^{\frac{-i\hat{H}}{\hbar}t}\Psi(x,0) \tag{5.1}$$

The operator $e^{\frac{-i\hat{H}}{\hbar}t}$ shows the evolution of the wave-function from time, 0, to time, t [Sen14]. This is expressed as $\hat{U}(t)$, or more specifically $\hat{U}(t,t_0)$, taking into account an initial time:

$$\hat{U}(t,t_0) = e^{\frac{-i\hat{H}}{\hbar}(t-t_0)} \tag{5.2}$$

This allows $\hat{U}$ to operate over all time, not just from 0 to t. In a physical context the time operator is useful in evolving to find the past and future of a wave-function.

5.2 Matrix Exponentiation

The time evolution operator should strike a concern. There is a matrix in the exponential. Results from the TDSE have brought about a supposed mathematical impossibility. Hence, in the early 1900s, linear algebra adapted with Lie theory, allowing for matrix exponentiation [Col14]. Unfortunately, Lie theory is well beyond this essay. Nevertheless, a simple definition of matrix exponentiation can be found from the Taylor series decomposition of e^x.

$$e^x = \exp(x) = 1 + x + \frac{x^2}{2!} + \frac{x^3}{3!} + \cdots = \sum_{k=0}^{\infty} \frac{x^k}{k!} \tag{5.3}$$

It is at this point we can differentiate between e^x and the function $\exp(x)$. For real values, it makes sense to call $\exp(x)$ as e^x, since powers of numbers are well defined on $\mathbb{R}$. However, for complex numbers and matrices, this doesn't mean anything. Hence, literature often refers to e^x as $\exp(x)$ since the Taylor series decomposition is the true definition, consistent for real values, complex values, and matrices [San20]. Hence, for a matrix, M [Kla19]:

$$\exp(M) = I + M + \frac{M^2}{2!} + \frac{M^3}{3!} + \cdots = \sum_{k=0}^{\infty} \frac{M^k}{k!} \tag{5.4}$$

This could be proved to converge for all complex matrices, but it is much easier to prove for the Hamiltonian matrix which is diagonalisable. Diagonalisation of the Hamiltonian requires a transformation matrix which only works if the Hamiltonian has a basis which spans the entire Hilbert space. Since the Hamiltonian is Hermitian, it spans the Hilbert space with an orthonormal basis. Hence it works to prove the exponent definition converges for diagonal matrices.

Let matrix, $D =$

$$\begin{bmatrix} d_1 & 0 & \cdots & 0 \\ 0 & d_2 & \cdots & 0 \\ \vdots & \cdots & \ddots & 0 \\ 0 & \cdots & 0 & d_n \end{bmatrix}$$

Using Eq. 5.4:

$$\exp(D) = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \cdots & \ddots & 0 \\ 0 & \cdots & 0 & 1 \end{bmatrix} + \begin{bmatrix} d_1 & 0 & \cdots & 0 \\ 0 & d_2 & \cdots & 0 \\ \vdots & \cdots & \ddots & 0 \\ 0 & \cdots & 0 & d_n \end{bmatrix} + \begin{bmatrix} \frac{d_1^2}{2!} & 0 & \cdots & 0 \\ 0 & \frac{d_2^2}{2!} & \cdots & 0 \\ \vdots & \cdots & \ddots & 0 \\ 0 & \cdots & 0 & \frac{d_n^2}{2!} \end{bmatrix} + \cdots$$

$$\exp(D) = \begin{bmatrix} e^{d_1} & 0 & \cdots & 0 \\ 0 & e^{d_2} & \cdots & 0 \\ \vdots & \cdots & \ddots & 0 \\ 0 & \cdots & 0 & e^{d_n} \end{bmatrix} \tag{5.5}$$

To rigorously complete the proof that diagonalisation and exponentiation works, consider diagonalisable matrix, M. M is diagonalised using the transformation matrix, X, such that $X^{-1}MX$ is diagonalised. After exponentiating the matrix, it can be transformed back by applying the operations in reverse. Hence:

$$\exp(M) = X \exp\bigl(X^{-1}MX\bigr)X^{-1} \tag{5.6}$$

This can be confirmed using Eq. 5.4. Consider a rearrangement of Eq. 5.6:

$$\begin{aligned}
X^{-1}\exp(M)X &= \exp\bigl(X^{-1}MX\bigr) \\
&= I + X^{-1}MX + \frac{(X^{-1}MX)^2}{2!} + \cdots \\
&= I + X^{-1}MX + X^{-1}\frac{M^2}{2!}X + \cdots \\
&= X^{-1}(I + M + \frac{M^2}{2!} + \cdots)X \\
&= X^{-1}\exp(M)X
\end{aligned}$$

For any diagonalisable complex matrix, M, there is a convergent solution to the matrix exponential [Kla19], shown by Eq. 5.6. The connection between the abstractness of the Hilbert space and an actual time evolver is once again, remarkable.

5.3 Application

After acquiring Eq. 5.1, it is important to demonstrate the equation in the context of an example with numerical values. To do so, the Hamiltonian needs to be expressed in terms of the possible energy measurements (eigenvalues). The following steps utilise Eq. 4.5 [Lit19].

$$\begin{aligned}
\Psi(x,t) &= \exp\left(\frac{-i\hat{H}}{\hbar}t\right)\Psi(x,0) \\
\Psi(x,t) &= \sum_{n=1}\exp\left(\frac{-i\hat{H}}{\hbar}t\right)b_n\varphi_n(x,0) \\
\Psi(x,t) &= \sum_{n=1}b_n\exp\left(\frac{-i\hat{H}}{\hbar}t\right)\varphi_n(x,0)
\end{aligned}$$

This expresses the wave-function in terms of its eigenstates, allowing the Hamiltonian to be evaluated on the n-th eigenstate. Noting the TISE: there are n eigenvalues, E_n, for each individual eigenstate, φ_n. Hence, the equation above can be rewritten:

$$\begin{aligned}
\Psi(x,t) &= \sum_{n=1} b_n(1 + (-it/\hbar)\hat{H} + \frac{(-it/\hbar)^2}{2!}\hat{H}\hat{H} + \cdots)\varphi_n(x,0) \\
\Psi(x,t) &= \sum_{n=1} b_n(\varphi_n(x,0) + (-it/\hbar)\hat{H}\varphi_n(x,0) + \frac{(-it/\hbar)^2}{2!}\hat{H}\hat{H}\varphi_n(x,0) + \cdots) \\
\Psi(x,t) &= \sum_{n=1} b_n(\varphi_n(x,0) + (-it/\hbar)E_n\varphi_n(x,0) + \frac{(-it/\hbar)^2}{2!}E_n^2\varphi_n(x,0) + \cdots) \\
\Psi(x,t) &= \sum_{n=1} b_n(1 + (-it/\hbar)E_n + \frac{(-it/\hbar)^2}{2!}E_n^2 + \cdots)\varphi_n(x,0) \\
\Psi(x,t) &= \sum_{n=1} b_n e^{\frac{-iE_n}{\hbar}t}\varphi_n(x,0) \\
\Psi(x,t) &= e^{\frac{-iE}{\hbar}t}\Psi(x,0) \qquad (5.7)
\end{aligned}$$

For any system with a set of energy eigenvalues, the wave-function can be solved for in terms of the corresponding eigenstates and eigenvalues. It is interesting to see that Eq. 5.7 ties in to the original wave-function definition in Eq. 2.8.

$$\Psi(x,t) = e^{\frac{-iE}{\hbar}t}\Psi(x,0) = e^{-i\omega t}\Psi(x,0) = e^{-i\omega t}e^{ikx} = e^{ikx-iwt}$$

After using simple calculus to derive equations that model the evolution of the wave-function, and using concepts from Lie theory, the final result is the wave-function itself. This shows that the theory is mathematically and physically consistent throughout, confirming the ansatz's accuracy.

As for an application, consider the superposition of a system, β [Lit19].

$$|\beta\rangle = \frac{1}{\sqrt{2}}|0\rangle + \frac{1}{\sqrt{2}}|2\rangle \qquad (5.8)$$

$|\beta\rangle$ is the wave-function with eigenstates, $|0\rangle$ and $|2\rangle$. The coefficients of the eigenstates satisfy the conditions outlined in Section 4.8. Assume that the associated eigenvalues for each eigenstate are: $E_0 = \hbar\omega/2$, $E_2 = 5\hbar\omega/2$. Hence $\beta(t)$ can be represented as such:

$$
\begin{aligned}
|\beta(t)\rangle &= \frac{1}{\sqrt{2}} e^{\frac{-i\hat{H}}{\hbar}t} |0\rangle + \frac{1}{\sqrt{2}} e^{\frac{-i\hat{H}}{\hbar}t} |2\rangle \\
|\beta(t)\rangle &= \frac{1}{\sqrt{2}} e^{\frac{-iE_0}{\hbar}t} |0\rangle + \frac{1}{\sqrt{2}} e^{\frac{-iE_2}{\hbar}t} |2\rangle \\
|\beta(t)\rangle &= \frac{1}{\sqrt{2}} e^{\frac{-i\hbar\omega/2}{\hbar}t} |0\rangle + \frac{1}{\sqrt{2}} e^{\frac{-5i\hbar\omega/2}{\hbar}t} |2\rangle \\
|\beta(t)\rangle &= \frac{1}{\sqrt{2}} e^{-i\omega t/2} |0\rangle + \frac{1}{\sqrt{2}} e^{-5i\omega t/2} |2\rangle
\end{aligned}
$$

A very curious result here is that $e^{-i\omega/2}$ and $e^{-5i\omega/2}$ cannot merge with the coefficient to their left. If this occurred, the fundamental eigenvalues of this system would change, which is impossible. If a system can either have energy E_0 or E_2, it cannot suddenly have an intermediary energy after a certain time. This would be considerably problematic for electron energy levels, which are discrete and have an absolute energy value. Hence, the $e^{-i\omega/2}$ and $e^{-5i\omega/2}$ merge with the two eigenstates [Cap12]. This is confusing since the eigenstates were not meant to change with time. However, $e^{-i\omega/2}$ and $e^{-5i\omega/2}$ are only phase **factors** for the eigenstates. Only phase **shifts** can change the overall probability of a function. Hence, the eigenstates themselves remain the same [Voo05]. The mathematics remains true to physical results, even if supposedly contradictory at first.

5.4 Inconsistency with Relativity

Clearly QM is mathematically sufficient in describing small-scale systems. However, this essay would be incomplete without considering inconsistencies with general relativity. Firstly, probabilistic descriptions of QM broke fundamentals in deterministic classical physics [Mam15]. The TDSE also assumed the existence of an absolute global time and an absolute state of reference [MC08]. Both of these mathematical results are inconsistent with the propositions of general relativity. That isn't to say that the mathematics itself is flawed. Literature would indicate that while there are contradictions introduced in the mathematics, both fields of physics can be practically analysed without issue, accounting for errors [XP16]. This points to a failure in physical understanding, but a certain versatility in mathematics as a tool.

6 Conclusion

Differential calculus, and more importantly, linear algebra, are often challenged by academic communities in their necessity in creating sufficient scientific models. This essay delves into the usage of mathematics in the development of QM in the early 1900s. The foundation of describing particles in QM is discussed with reference to Euler's form, and then linear algebra is selected as a mathematical structure to support problems in QM. The results are shown to be consistent, both mathematically (in comparison to the original wave-function) and physically (in application to real problems).

Furthermore, this essay humours the fundamental question of the necessity of the application of abstract mathematics in describing the real world. Abstract mathematics, while “imaginary”, is accurate and surprisingly convenient when considering the functionality of the Schrodinger's equations. While it is important to consider alternate explanations and motivations for QM, shown in QED by Feynman, the mathematics discussed in this essay sacrifice no ability to be versatile and accurate.

Admittedly, this essay would benefit from a consideration of a variety of other mathematical methods of QM, especially Lie theory and Feynman's alternative to complex numbers. Assessing different mathematical tools would provide a more comprehensive resolution to the question.

References

[Alf08] Mark Alford. "The Essentials of Quantum Mechanics". In: *A few pieces of physics* (Oct. 2008). URL: `https://web.physics.wustl.edu/alford/physics/`.

[Bee17] Robert Beezer. "Linear Transformations". In: *A First Course in Linear Algebra* (Apr. 2017). URL: `http://linear.ups.edu`.

[BH20] Seymour Blinder and David Hanson. "3.3: The Schrödinger Equation is an Eigenvalue Problem". In: *Chemistry LibreTexts* (Jan. 2020). URL: `https://chem.libretexts.org`.

[Cap12] Paola Cappellaro. "6. Time Evolution in Quantum Mechanics". In: *Introduction to Applied Nuclear Physics MIT OCW* (2012).

[Col14] Brenden Collins. "An Introduction to Lie Theory Through Matrix Groups". REU. University of Chicago, 2014.

[Dir58] Paul Adrien Maurice Dirac. *The Principles of Quantum Mechanics.* 4th ed. Oxford University Press, 1958. Chap. 1. ISBN: 9780198520115.

[Dwo] Maria Dworzecka. "The Superposition Principle". In: *Lecture Notes GMU* (). URL: `http://physics.gmu.edu`.

[Fey85] Richard Feynman. *QED: The Strange Theory of Light and Matter.* Princeton University Press, 1985. ISBN: 9780691024172.

[Gri04] David Griffiths. *Introduction to quantum mechanics.* 2nd ed. Pearson Prentice Hall, 2004. Chap. 3. ISBN: 9780131118928.

[Hee] David Heeger. "Linear Systems Theory". In: *Lecture Handouts* (). URL: `https://www.cns.nyu.edu`.

[HH20] Erica Harvey and David Hanson. "11.10: The Schrödinger Wave Equation for the Hydrogen Atom". In: *Chemistry LibreTexts* (Jan. 2020). URL: `https://chem.libretexts.org`.

[Kar19] Ricardo Karam. "Why are complex numbers needed in quantum mechanics? Some answers for the introductory level". In: *American Journal of Physics* 88 (1 Dec. 2019).

[Kla19] Dan Klain. "The Matrix Exponential and Linear Systems of ODEs (with exercises)". In: *Department of Mathematical Sciences, University of Massachusetts Lowell* (Oct. 2019).

[Lit19] Robert G. Littlejohn. "Notes 5: Time Evolution in Quantum Mechanics". In: *UC Berkeley Physics 221A* (2019).

[Mam15] Aghaddin Mamedov. "Unification of Quantum Mechanics with the Relativity Theory, Based on Discrete Conservations of Energy and Gravity". In: *Selected Topics in Applications of Quantum Mechanics*. Ed. by Mohammad Reza Pahlavani. Mazandaran: University of Mazandaran, May 2015. Chap. 4.

[MC08] Alfredo Macías and Abel Camacho. "On the incompatibility between quantum theory and general relativity". In: *Physics Letters B* 663 (May 2008), pp. 99–102.

[Nav16] C.R. Nave. *The Hamiltonian*. 2016. URL: `http://hyperphysics.phy-astr.gsu.edu/hbase/quantum/hamil.html`.

[Neu55] John von Neumann. *Mathematical Foundations of Quantum Mechanics*. Ed. by Nicholas A. Wheeler. Trans. by Robert T. Beyer. Princeton University Press, 1955. Chap. 1. ISBN: 9780691178561.

[Qua12] Saad Quader. “Eigenvalues of a Hermitian Matrix are Real”. In: *Elementary, Expository, Mathematics, Matrix Analysis* (Nov. 2012). URL: `https://saadquader.wordpress.com`.

[Qua16] Saad Quader. “In a Hermitian Matrix, the Eigenvectors of Different Eigenvalues are Orthogonal”. In: *Elementary, Expository, Mathematics, Matrix Analysis* (Sept. 2016). URL: `https://saadquader.wordpress.com`.

[Qui+14] Catherine Quinn et al. *Further Mathematics HL: Linear Algebra and Geometry*. 2014. Chap. 1.

[San20] Grant Sanderson. *What is Euler’s formula actually saying? — Lockdown math ep. 4*. Youtube. 2020. URL: `https://www.youtube.com/watch?v=ZxYOEwM6Wbk`.

[Sch16] Daniel V. Schroeder. “2. Wavefunctions”. In: *Weber State University - Quantum Mechanics (Physics 4610)* (2016).

[Sch26] Erwin Schrodinger. *Schrödinger to Lorentz*. Zurich, June 1926.

[Sen14] Rajdeep Sensarma. “Lecture 9: Quantum Dynamics”. In: *Tata Institute of Fundamental Research: Advanced Quantum Mechanics* (2014).

[Sim09] Ben Simons. *Lecture notes in Advanced Quantum Mechanics*. University of Cambridge, Nov. 2009. Chap. 3.

[Voo05] Troy Van Voorhis. “V. Time Dependence”. In: *Introductory Quantum Mechanics I MIT OCW* (2005).

[Wei20a] Eric Weisstein. “Eigenvector”. In: *Wolfram* (Jan. 2020). URL: `http://mathworld.wolfram.com`.

[Wei20b] Eric Weisstein. “Hermitian Matrix”. In: *Wolfram* (Feb. 2020). URL: `http://mathworld.wolfram.com`.

[Wig60] Eugene Wigner. “The Unreasonable Effectiveness of Mathematics in the Natural Sciences”. In: *Communications in Pure and Applied Mathematics* 13 (1 Feb. 1960).

[XP16] Ricardo Ximenes and Fernando Parisio. “Quantifying the failure of Schrödinger dynamics in the free expansion of relativistic particles”. In: *The European Physical Journal Plus* 131 (Nov. 2016).

[Zwe16a] Barton Zweibach. “Lecture 1: Quantum Physics I”. In: *Massachusetts Institute of Technology - Open Courseware* (Feb. 2016).

[Zwe16b] Barton Zweibach. “Lecture 3: Quantum Physics I”. In: *Massachusetts Institute of Technology - Open Courseware* (Feb. 2016).

[Zwe16c] Barton Zweibach. “Lecture 4: Quantum Physics I”. In: *Massachusetts Institute of Technology - Open Courseware* (Feb. 2016).

[Zwe16d] Barton Zweibach. “Lecture 5: Quantum Physics I”. In: *Massachusetts Institute of Technology - Open Courseware* (Feb. 2016).