Mathematical Quantum Mechanics

MATH 470 Final Report

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Abstract. In this project, we seek to provide an introduction to a rigorous formulation of quantum mechanics aimed at mathematicians.

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1. Introduction

Quantum mechanics is the theory of physics we used to describe physics at small (atomic and subatomic) scales. These are the the scales where classical mechanics as we know it breaks down. There are numerous key features that distinguish quantum mechanics from classical mechanics. The first feature is the *discretization* of quantities that we measure in systems, such as energy and momentum. This restriction to a set of discrete values is called **quantization**. In this theory of physics, we also see that all objects share both wave and particle characteristics. This dual-nature of objects is called **wave-particle duality**. Finally, the most shocking claim made by quantum mechanics is that nature is inherently random; in other words, there are limits to how much of a physical quantity (such as position and momentum) that we can predict prior to making a measurement. This phenomenon is called the **uncertainty principle**.

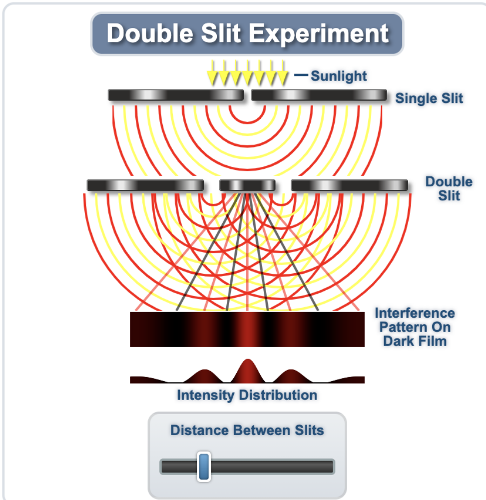
We will first begin this report by providing a historical background, in Section 2. Then, in Section 3 we provide a mathematical formulation of classical mechanics. In section 4 we begin introducing the key ideas of mathematical quantum mechanics. In Section 5 we provide a brief introduction to the Fourier Transform, a mathematical object which plays a central role in quantum mechanics. In Section 6 we present all the axioms of quantum mechanics. Finally, we end the paper by discussing the spectral theory and its application to Schrödinger operators in Section 7.

2. Historical Background

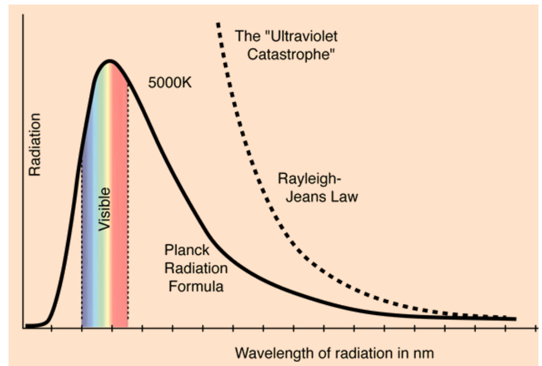
The first potential cracks in the theories of classical mechanics appeared in the late 1600s to early 1700s in the midst of a debate in the scientific community over the nature of light. Physicists were split into two main camps: those who agreed with Issac Newton, who argued that light was a collection of particles, and those who agreed with Christiaan Huygens, who argued that light was a wave. In part due to Newton's clout in the scientific community, at the time the general scientific consensus at the time was that light is a wave.

It was not until Thomas Young's double slit experiment in 1804 when the status of light as a collection of particles was questioned. In this experiment, as pictured in Figure 1a, Young observed sunlight pass through two small holes in a cardboard box. The pattern observed on the dark film strongly suggested that light was a wave; the distinctive interference patterns observed on the film would be impossible if light was only a collection of particles. This observation, along with numerous other experiments at the time (including Maxwell's experiments which predicted that electromagnetic waves propagate at the same speed which was observed for light) shifted the general scientific consensus from favouring a particle-centric theory of light to a wave-centric theory of light. This wave theory of light remained the scientific consensus until the end of the 19th century.

However, this consensus did not last for long. In 1900, Planck's model of blackbody radiation (see Figure 1b) sparked the rebirth of the particle theory of light once more. In short, if light was not a collection



(a) Cartoon depiction of Thomas Young's double slit experiment in 1804.



(b) Planck's model of blackbody radiation.

Figure 1

of particle, then the equipartition theory of statistical mechanics predicted what was called the **ultraviolet catastrophe** — a phenomena whereby a blackbody releases an arbitrarily high amount of energy, resulting in all matter instantaneously radiating all of its energy until its energy approaches absolute zero. This was obviously very problematic, since this clearly deviates from empirical observations. Planck was able to solve this catastrophe by *discretizing light's energy.* In particular, Planck assumed that the emission and absorption of electromagnetic radiation could only occur in discrete packets – called **quanta** – of energy. This relationship was encoded in the following formula relating the energy of a quanta to the frequency of light,

$$E_{\text{quanta}} = h\nu, \tag{1}$$

where $h = 6.63 \times 10^{-34}$Js is **Planck's constant** and ν is the frequency of light.

Albert Einstein's observation of the photoelectric effect in 1921, which earned him his Nobel prize, provided even more evidence for a particle-like nature of light. In this experiment, a light ray was shot at a sheet of metal. During this procedure, electrons are emitted from the metal. In short, the experimental results that were observed would be absolutely puzzling if light was purely a wave. In particular, a wave theory of light would predict that as the intensity of the light increased, the energy of the emitted electrons should increase accordingly. This was not observed – rather, the *number* of emitted electrons changed as the intensity of the light changed. With both sides of the wave-particle debate about the nature of light amassing sufficient evidence, the concept of **wave-particle duality** was born: light was both a wave and a collection of particles.

It wasn't long until the status of electrons, and consequently matter in general, was also thrown into question. *Is an electron a wave or a particle?* Before the late 19th century, there was no reason to believe that an electron was nothing more than a particle. However, the study of the atomic structure in the late 19th and early 20th century ushered in an uncomfortable question: could matter actually be a wave? This question is illustrated by the study of the hydrogen atom. As electron is shot at a cloud of hydrogen gas, the electrons in each hydrogen atom become excited. In this process, the jump into a higher energy state. After some time, the electron will return to its ground energy state and in the process emit a photon. In the late 1800s, physicists observed this behaviour, and noted that these emitted photons, and consequently the energies of a hydrogen atom, only came in a discrete set of values. Johannes Rydberg computed this set of values,

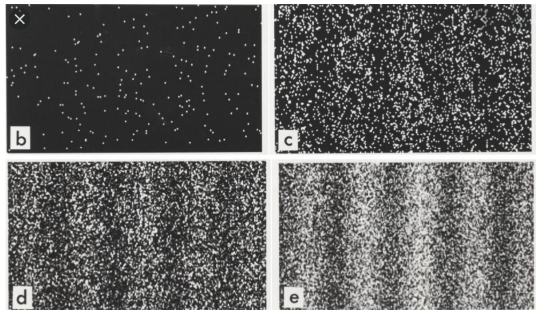


Figure 2. Double slit experiment in 1989 for electrons.

explicitly

$$E_n = -\frac{R}{n^2} \text{ where } R = \frac{m_e Q^4}{2\hbar^2}, \tag{2}$$

where R is the Rydberg constant, n is some natural number, m_e is the rest mass of the electron, Q is the charge of the electron, and $\hbar$ is the reduced Planck's constant, which is related to Planck's constant by $\hbar = \frac{h}{2\pi}$. Using these values, Rydberg computed the observed frequencies of the hydrogen atom to be of the form

$$\omega = \frac{1}{\hbar}(E_n - E_m) \text{ where } n > m. \tag{3}$$

We call Equation 3 the **spectrum** of the hydrogen atom. This puzzling observation would remain a mystery until the theory of quantum mechanics was formulated in the 20th century. In 1989, the famous double slit experiment for electrons (pictured in Figure 2) provided more evidence for a wave-like nature of electrons. Note that the same interference patterns which were observed for light are present for matter; this led to the concept of wave-particle duality for matter. Everything now exhibits wave-particle duality!

In 1926, Born precisely formulated the concept of randomness in quantum with his **Copenhagen interpretation of quantum mechanics**. We can understand this by contrasting quantum mechanics to classical mechanics. In classical mechanics, everything is deterministic: given information about a particle's spatial location and momentum (which we can solve for using Newton's second law), we can make any prediction we'd like about a particle. In quantum mechanics, this is not true. Instead, the objective is not to solve $\mathbf{F} = m\mathbf{a}$; instead, we have to solve a partial differential equation – Schrödinger's equation – for a wave function $\Psi(x,t)$. Squaring the absolute value of the wave function, $|\Psi(x,t)|^2$, we do not get a deterministic set of predictions. Instead, we get a probability distribution function for where the particle *might* be. Potential values for the particle's momentum are encoded in the frequency of $|\Psi(x,t)|^2$. As we will see later, these two observables will be related by a mathematical object called the fourier transform.

3. Mathematical Formulation of Classical Mechanics

4. Foundations of Mathematical Quantum Mechanics

5. Math Detour: Fourier Transform

6. Axioms of Quantum Mechanics

7. Spectral Theory and Schrödinger Operators

References