Exploring Quantum Mechanics and the Schrödinger Equation

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Contents

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1 Abstract

Quantum mechanics is the study of matter and energy on the smallest scales of subatomic particles. Through various experiments in the early twentieth century, it was shown that at this level the laws of classical physics no longer held true, so a new model was needed to explain the discrepancies that had arisen.

This article explores the strange world of quantum mechanics, one strand of this physics revolution, with a particular focus on the Schrödinger equation and the discoveries leading up to it. We explain how the equation was derived, what it represents, and use it to model solutions to a number of different potential scenarios. We hope to show how quantum mechanics differs from classical physics, as well as the real life applications of the field.

2 Introduction

By the beginning of the twentieth century, classical physics had been established as the key to determining all the workings of the natural world. The consensus was that any further modifications would only add minor improvements to the physical model. However, there remained a number of inexplicable observed facts about the universe; the questions these raised would subsequently motivate an entirely new way to describe and model the world around us.

These were important questions, not the spawn of theoretical scenarios. The inconsistencies uncovered by these experimental results threatened to dismantle established laws of physics. They exposed classical physics' predictions for fundamental aspects of the world as blatantly wrong. The atom does not collapse upon itself, and the Sun does not radiate infinitely intense gamma rays. Furthermore, the discrepancies between predicted and actual outcomes challenged ideas about the world on an axiomatic level, and these were even more disruptive. Waves and particles were no longer so different, and scientists had to grapple with an inherent uncertainty. The resolution of this existential crisis in physics was found in the quantum revolution[1].

Our paper will follow this transformation of physics in the early twentieth century, outlining the inconsistencies that toppled established norms, and the developments of physicists like Planck, Einstein, and Schrödinger in settling them. Our aim is to digest and explain the conceptual leaps bridging the classical and quantum interpretations of nature in an accessible way, being mindful of quantum mechanics' reputation as impenetrable and unintuitive. We will derive Schrödinger's equation and apply it to multiple theoretical scenarios, exploring the consequences of its solutions. This should give us further insight into the physical use of quantum effects.

Some of the last century's defining technological advancements and most exciting experimental research came as a result of quantum mechanics, revolutionising our scientific outlook on the world. It has allowed us to manipulate the smallest and most basic level of all there is, rapidly accelerating our electrical capabilities[2]. This minute control has enabled the digital era and the technology now essential in our everyday lives. In our project, we will explore some of the key applications of quantum mechanics and examine future possibilities in quantum computing.

In order to begin exploring these unfamiliar ideas, we first had to establish a solid foundation of some required mathematical material. This stage was crucial as almost all of the calculations in quantum mechanics require tools from calculus and numerical analysis, areas that we had not encountered to a great extent. In parallel with this, due to the unintuitive nature of quantum mechanics, we needed to devote much of our attention to accustom ourselves to the key concepts of the field and its differences to a classical interpretation. It felt natural, therefore, to follow the history of its early development, from Planck's solving of the ultraviolet catastrophe[3] right up to the emergence of Schrödinger's equation. We mapped out the progression of these ideas, and how each precipitated the next.

3 Literature Review

Quantum mechanics is one of the few truly revolutionary progressions in physics. Just as Newton laid a foundation for classical mechanics and Einstein's relativity encompassed classical physics as a limiting case, quantum mechanics shifted the axioms through which twentieth century physicists and their successors viewed the world. Since we were approaching this project having only encountered classical physics, it was necessary to first research the main deviations from this physical model. We therefore decided to begin studying experimental results that exposed inconsistencies in classical physics before delving into the technicalities of Schrödinger's equation. From a position of unfamiliarity, these key concepts required us to devote adequate time to them at the beginning of our project.

We decided to first explore Bohr's model of the atom and how physicists' understanding of atomic particles changed during the quantum revolution, as this bridges the classical and quantum representations. While Bohr's model is incomplete and does not incorporate wave-particle duality, it was the first significant introduction of the quantisation of energy into physics.

To this end, we studied the article 'The Bohr Model of the Atom'[4] by Niels Walet, a professor of classical physics at the University of Manchester. As well as years of experience in a relevant field, he also has extensive experience with writing online learning resources which therefore makes this source reliable and highly accessible to our group. The article goes into a brief history of the structure of the atom, and contextualises the quantum developments within a larger historical timeline. It gives an adequate introduction to the Bohr model of the atom, explaining how energy quantisation changed the atomic picture, and introduces discrete electron energy levels. However, Walet gives only an intuitive overview of these topics and does not emphasise the links to the focus of our project, so it was necessary to find further, more relevant sources. This source was useful to our group as we explored how quantum mechanics elucidates the Bohr model of the atom, although we chose not to study it thoroughly as it is only an introductory resource. Furthermore, this piece is part of a large project, hence it mentions unfamiliar concepts, many of which are irrelevant to our project. As a result, we decided we needed to find sources more relevant to our specific brief, drawing upon more concepts from quantum mechanics.

We therefore next looked at an online article by Gordon Squires[5] that explores the developments succeeding Bohr's model that accelerated the quantum revolution. Gordon details the discoveries that laid the foundations for the modern understanding of quantum mechanics and briefly refers to some of its key premises. He reviews some of the fundamental ideas in the field, namely the photoelectric effect, Bohr's model of the atom, as well as de Broglie and Schrödinger's interpretations of wave mechanics. The article focuses on investigations of the atom such as the gold leaf experiment and the subsequent discoveries it led to, specifically Rutherford's and Bohr's alterations to the atomic model. Squires also gives a cursory review of Planck's hypothesis and Schrödinger's equation. He describes the journey of these discoveries being made, and how empirical evidence from experiments like the gold leaf experiment inspired new ideas that challenged the existing physical model. This clear structure was useful for our research as it helped us gain a deeper understanding of the core ideas underpinning the subject. Squires is a lecturer in physics at the University of Cambridge and has written other publications on quantum mechanics[6] , which lends him credibility. The main limitation of the article is its failure to mention some of the key observations that were crucial in the development of the field such as the ultraviolet catastrophe and the electron double slit experiment. Therefore, it could only supply us with a basic understanding of the history leading to the quantum revolution and a brief introduction to some of its core concepts. This meant that further in-depth research would need to be carried out on the topics presented in this article.

At this point, we chose to study a more mathematically rigorous source for an explanation of the key notions of quantum mechanics and developments of the 1920s. David Morin's 'Introduction to Quantum Mechanics'[7] lecture notes walk the reader through the historical chronology of the quantum revolution and the derivation of Schrödinger's equation. He explains advancements like the discovery of wave-particle duality and introduces the wave function as a complex representation of a particle that gives its probability distribution. On the more technical side, he also presents a concise and detailed derivation of the Schrödinger's equation. This includes explained steps, for example how the kinetic energy of a particle is expressed in terms of the particle's momentum. David Morin is the senior lecturer on physics at Harvard University, with multiple other related publications and a PhD in theoretical physics from Harvard University. These qualifications make him an established authority hence this is a reliable source for our project. These notes were very valuable in our initial research into Schrödinger's equation and the wave function since it clearly presents the chronology of the quantum developments of the 1920s. Morin gives a detailed, well-structured introduction, which made it a good starting point for our research. The lecture notes are intended for readers who have preliminary knowledge of classical mechanics as it builds on this understanding to incorporate quantum concepts. This is its main limitation: readers are required to have a certain level of mathematical skills to follow much of the explanation and working. Therefore, we had to find additional supplementary materials for a more detailed and rounded understanding of this source.

Dr. Elwyn Elm's Article, 'Schrödinger's Probability Wave Equation'[8] is more focused on the concepts and interpretation of the early quantum developments than the mathematical details. He describes the role of Schrödinger's equation as encapsulating probabilities. Interestingly, Schrödinger himself disliked his work being portrayed this way. The wave function, which is what he was aiming to derive, represents the probabilities of the characteristics of a particle being a certain way at a given time. Yet, paradoxically, it does not involve uncertainty, since the wave function is described to be just as deterministic as Newton's equations of motion and gravitation. In other words, given enough parameters and conditions, Schrödinger's equation will predict precisely what the wave function will be at any future time. The departure from determinism instead is due to the shift from a particle occupying a point in space to being distributed throughout space, with a probability distribution for where it could be found. Elm also mentions an interesting part of history regarding the equation: in the mechanics arising from Schrödinger's equation, energy passes continuously from one vibration pattern to another, so what looks like a particle becomes a superposition of thousands of waves, which supports de Broglie's hypothesis of wave-particle duality. The key insight from this article for us was how theoretical the wave function really is; Elm states that the waves which are described by the equation are permanently and completely unobservable. This description of the departures of the quantum model from our intuitive grasp of the world allowed us to approach and better understand the nature of Schrödinger's equation. Dr Elm has received a doctorate in philosophy and has experience in the field of law with a multitude of publications, making him an established academic writer. However, since these are such disparate fields from physics, there are grounds to question the reliability of the article. The primary focus of the article is to give the reader an intuitive understanding around Schrödinger's equation and we therefore mainly used this source solely for supplementary information and background research, rather than a key learning resource.

At this point, we thought it would be useful to explore some alternative interpretations of Schrödinger's equation, to obtain a more rounded understanding of its key ideas. In his short paper 'Euler's formula is the key to unlocking the secrets of quantum mechanics'[9], Bichara Sahely introduces the wave mechanics of Schrödinger's wave equation, exploring the link with Euler's formula. Through comparison to electromagnetic waves as similarly helical waves, Sahely attempts to expose links between the different fields of physics. He concludes that the focus should be directed more towards finding the pattern that unites the unknown aspects of physics with the established known areas. While the content is highly relevant to our brief, namely understanding the meaning of the wave function, it is only a cursory overview of the topic, focused more on the link with other areas of physics and mathematics than the fine details of Schrödinger's equation, aimed at an audience that is more casually interested than students in want of detailed explanation. Furthermore, even though Bichara Sahely was a professor at the University of Toronto, he is a doctor of Internal Medicine and now a private physician consultant. This means he is perhaps an unreliable source in the field of physics, having never done any research work himself in the subject. However, this outside perspective was possibly more useful to us than a highly technical description from a professional's point of view, due to the more intuitive and hence accessible writing. This source was only useful to our group as a supplementary overview and possibly a different way to interpret Schrödinger's equation, but not as a learning resource.

Our preliminary research into quantum mechanics provided us with a greater appreciation of the alterations from the classical model, giving us a basic understanding of Schrödinger's equation and the wave function. This knowledge formed a foundation upon which we could conduct further research with confidence. We found that our sources focused primarily on the explanations of the concepts but lacked detail on mathematical material that could be applied for calculations. Solving Schrödinger's equation would require the application of technical tools that were unfamiliar, such as calculus and solving differential equations. Therefore, we needed to continue developing the relevant mathematical skills, which would enable us to progress onto solving Schrödinger's equation in different theoretical scenarios, such as potential wells. To achieve this, we further studied David Morin's lecture notes, as these explain solutions and workings for such problems. However, we had to research other sources to reinforce our mathematical tool set as supplementary aids. Naturally, we would still draw upon the other resources detailed above for alternative explanations and interpretations of the concepts as we progressed and our final direction for the project crystallised.

4 Development and Methodology

4.1 Timeline of our work

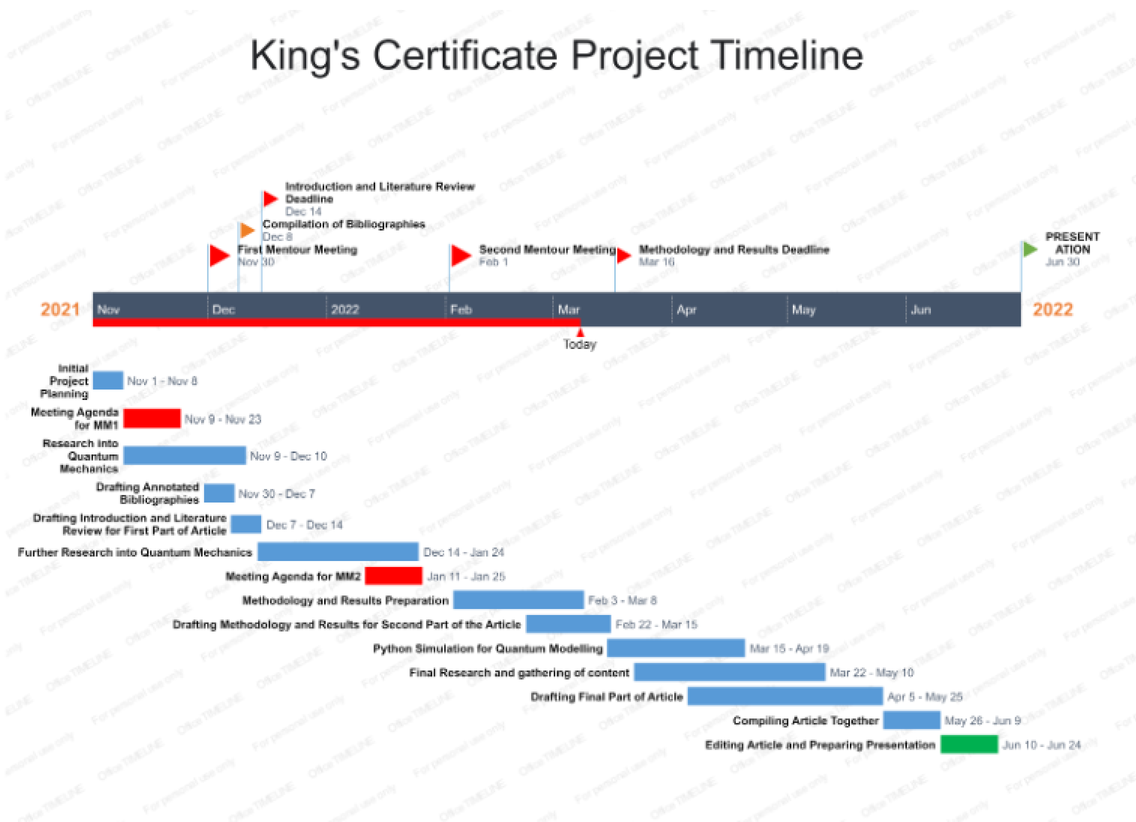

Figure 1: Gantt chart displaying our timeline of work

At the beginning of our project we drafted a plan, alongside a Gantt chart to guide us. Our focus was to obtain an intuitive understanding of quantum mechanics, and we firstly focused on the history of the field, exploring its synthesis when Planck resolved the ultraviolet catastrophe[10] up until Schrödinger derived his equation. A key priority for us was to write Python programs to generate graphs and plots for the quantum wave function, the heart of Schrödinger's equation, to better understand and visualise its meaning and behaviour. More informal sources proved to be more useful at the initial stage, since the complex mathematics involved made technical articles inaccessible to us at the time. To bridge this gap, we also began developing our elementary calculus skills - a crucial component to understanding Schrödinger's equation. Our initial introduction to more advanced material formed our literature review, as well as the derivations of the most used equations.

This was done in parallel with the continuation of our exploration into the key concepts distinguishing the quantum from the classical model, and investigating more specialised areas such as quantum computing, tunnelling[11], and Bohr's model of the atom. We reinforced our understanding of both of these areas in our first mentor meeting with Dr. Fenner Harper, which we found a fruitful opportunity to gain expert insight into these sometimes unintuitive ideas. After this meeting, we built upon this preliminary research, putting these concepts to use in deriving Schrödinger's equation, which we used to solve the infinite potential well. Each member on the group would have assigned areas to research with appropriate deadlines, the results of which would be discussed and reflected upon at our organised meetings, which happened approximately every two weeks.

Our second mentor meeting was more directed to formulating a final direction, and we decided that going forward we would explore the methods of applying Schrödinger's equation. We would do this by solving more complicated systems to find the wave function, with a focus on the differences to the classical model, such as the phenomenon of quantum tunneling. We aimed to complete a draft of our solutions by the end of May, a deadline we delivered on, which gave us a reasonable amount of time to review, edit, and finalise the article.

4.2 Wave-particle duality

The research we conducted as part of our literature review highlighted key concepts for understanding the equations and predictions of quantum mechanics. These were usually changes to classical ideas that resulted from experiments in the early twentieth century, and the most notable shift in perspective was seen in the principle of wave-particle duality. Waves and particles are not treated as distinct entities as in classical physics. Particles have wave-like properties and behaviours, no longer located at an exact point in space, but rather distributed throughout a region. These revolutionary ideas were developed in degrees as experimental inconsistencies with the classical model began to emerge.

One of the first major problems that challenged contemporary ideas of the early twentieth century arose when physicists attempted to explain the electromagnetic radiation from an ideal black-body. The equations of classical physics predicted that the intensity of emission would be inversely proportional to the wavelength, which would result in infinitely intense radiation of shorter wavelengths. Clearly, this is not what is seen in nature, and classical equations failed to explain the observed curve of intensity across the electromagnetic spectrum. Eventually, in 1901, the physicist Max Planck proposed a solution[12] that introduced the assumption that energy is emitted in discrete amounts, or 'quanta', defined by a constant now known as *Planck's constant*. With this assumption, the observed curve could be perfectly replicated.

It would be Einstein's work on the photoelectric effect[13] in 1905 that would extend this theory and explain its physical significance. Einstein found that when light of a sufficient frequency is incident on a metallic surface, electrons will be emitted. However, when the frequency of light gets below a certain threshold value, no photo-electrons are observed at all, showing that the energy the light transfers to the electrons is delivered in discrete 'energy packets'. This was evidence for the existence of the photon, a particle carrying electromagnetic waves, and represented the first time the boundaries between particles and waves had been challenged. The light behaves as a wave up until the point of interaction with the metal surface, at which point its behaviour is that of a particle. Einstein had incorporated Planck's theory, suggesting that the energy 'quanta' Planck described was in fact the photon. Until this point, physics had embedded continuous values into its models, and these ideas represented an uprooting of this, restricting the energy of emitted light to certain discontinuous levels.

However, the concept of wave-particle duality observed in the photoelectric effect was considered to be exclusive to light. This was extended in 1923 by Louis de Broglie in his doctoral dissertation[14], in which he claimed that all matter exhibited wave-like properties, and have an associated wavelength and frequency. He summarised this wave-particle duality in the relationships:

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

$$E = hf$$

where p and E are the momentum and energy of a particle respectively, λ and f are the wavelength and frequency of the associated wave respectively, and h is Planck's constant. Here, two quantities classically related to particles are directly equated to quantities classically related to waves. The quantum model treats the two interchangeably, with particles behaving like waves in certain situations and waves as particles in others. Something that seems intrinsically particulate like a proton is treated with the same equations governing vibrations on a string. Since Planck's constant is of the order of 10^{-34}, we do not observe the ideas of quantum mechanics on our scale, but on the level of sub-atomic particle, its equations make predictions that are equally accurate and counter-intuitive.

An example that demonstrates this idea clearly is the electron double slit experiment[15], conducted in 1961. More than a century before, Thomas Young had passed light through two slits onto a screen to prove its wave nature. The light diffracts as it passes through the aperture, spreading out and overlapping with the light from the other slit, resulting in characteristic interference patterns on the screen. This experiment was reproduced using electrons instead of light, and the same interference patterns were observed. This served as irrefutable evidence for wave particle duality: the electrons behaved as waves while they travelled through the slits towards the screen, but they interacted with the screen as particles. Moreover, when a single electron was passed through the slits, the same interference patterns emerged, suggesting the electron was able to interfere with itself. In the quantum world, a particle does not occupy a definite position or state, but can exist as a superposition of multiple different possibilities. The electron passed through both slits simultaneously, in a *superposition* of the two states, and it only collapsed into one once it interacted with the screen. This is called the *measurement problem*, since all of the information defining the particle's state, called the *wave function* can never be directly measured. The particle will collapse into one its possible states whenever an observation is made.

Clearly, the implications of the wave-particle duality were too extreme to be incorporated into the classical model, and instead required a new set of governing equations. The entire conception of a particle required reinvention, and the pursuit for a theory that unified the experimental findings of the early twentieth century culminated in Schrödinger proposing his equation.

4.3 Derivation of Schrödinger's Equation

Since our project brief revolved so heavily around Schrödinger's equation, we decided it was necessary to deeply understand the equation's origins and derivation. This would allow us to interpret the equation's significance and the main differences with the classical model.

Since Schrödinger's equation is widely known, we found its time-dependent and time-independent forms from David Morin's publication on waves[7]. We decided to explore the equation in one dimension x, since this simplifies much of the mathematics involved and for systems involving more dimensions, the same method can be applied to each dimension respectively. The first observation we made was that, due to the presence of Planck's constant, we would need to incorporate ideas of wave-particle duality, equating quantities classically related to particles like momentum and energy to quantities classically related to waves like wavelength and frequency. From classical physics[16] we have that the total energy of a system is given by:

$$\text{Total Energy (E)} \;=\; \text{Kinetic Energy (K)} \;+\; \text{Potential Energy (P)}$$

So

$$E = K + V = \frac{1}{2}mv^2 + V(x) = \frac{p^2}{2m} + V(x) \tag{1}$$

We accept as true the fundamental equations of wave-particle duality[17] mentioned earlier:

$$p = \frac{h}{\lambda} \tag{2}$$

$$E = hf \tag{3}$$

The physical quantities present in Schrödinger's equation, however, are different from these. We therefore had to research and define the reduced Planck's constant $\hbar$, angular frequency ω, and a wave number k, which can be thought of as a wave's frequency in space. These are given by:

$$\hbar = \frac{h}{2\pi}$$

$$\omega, \text{ angular frequency} = 2\pi f$$

with units of radians per second

$$k, \text{ wave number (spacial frequency)} = \frac{2\pi}{\lambda}$$

corresponding to the number of wavelengths per 2π meters
Substituting Equations [2] and [3] into Equation [1], we get:

$$hf = \frac{(\frac{h}{\lambda})^2}{2m} + V(x)$$

$$\hbar\omega = \frac{\hbar^2 k^2}{2m} + V(x) \tag{4}$$

Using de Broglie's theory that every particle has an associated wave[18] we can define this wave as:

$$\Psi(x,t) = Ae^{i(kx-\omega t)} \tag{5}$$

taking the position and time as parameters, where A is constant. This is a standard expression for wave motion, but it should be noted that this wave exists in the complex plane, and is not solely rooted in real numbers but also has an imaginary component.

From this we can determine this wave's partial derivatives in x and t:

$$\begin{aligned}\frac{\partial}{\partial t}Ae^{i(kx-\omega t)} &= Ae^{i(kx-\omega t)}x - i\omega \\ &= -i\omega Ae^{i(kx-\omega t)}\end{aligned}$$

$$\frac{\partial}{\partial t}Ae^{i(kx-\omega t)} = -i\omega\Psi(x,t) \tag{6}$$

$$\begin{aligned}\frac{\partial}{\partial x}Ae^{i(kx-\omega t)} &= Ae^{i(kx-\omega t)}xik \\ \frac{\partial}{\partial x}ikAe^{i(kx-\omega t)} &= i^2k^2Ae^{i(kx-\omega t)} \\ &= -k^2Ae^{i(kx-\omega t)}\end{aligned}$$

$$\frac{\partial^2\Psi(x,t)}{\partial x^2} = -k^2\Psi(x,t) \tag{7}$$

If we multiply Equation [4] by $\Psi(x,t)$:

$$\hbar\omega\Psi(x,t) = \frac{\hbar^2k^2}{2m}\Psi(x,t) + V(x)\Psi(x,t) \tag{8}$$

Substituting in Equations [6] and [7], we get:

$$i\hbar\left(-i\omega\Psi(x,t)\right) = -\frac{\hbar^2}{2m}\left(-k^2\Psi(x,t)\right) + V(x)\Psi(x,t)$$

This gives us the time-dependent Schrödinger's equation

$$i\hbar\frac{\partial\Psi(x,t)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} + V(x)\Psi(x,t) \tag{9}$$

For static situations or for solutions that form standing waves, we can remove the time dependence from Schrödinger's equation. Since these are the only types of solutions we will be exploring in this paper, we will exclusively use the time-independent Schrödinger's equation.

To remove the time-dependence, we let $\Psi(x,t) = g(t)\psi(x)$:

$$i\hbar\frac{\partial g(t)\psi(x)}{\partial t} = -\frac{\hbar^2}{2m}\frac{\partial^2 g(t)\psi(x)}{\partial x^2} + V(x)g(t)\psi(x) \tag{10}$$

Since $\psi(x)$ does not depend on t and $g(t)$ does not depend on x,

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

We know g(t) is of the form $e^{-i\omega t}$ so $\frac{\partial g(t)}{\partial t} = -i\omega g(t)$

$$i\hbar\psi(x)\cdot -i\omega g(t) = -\frac{-\hbar^2}{2m}g(t)\frac{\partial^2\psi(x)}{\partial x^2} + V(x)g(t)\psi(x)$$

Cancelling g(t):

$$\hbar\omega\psi(x) = -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial^2 x} + V(x)\psi(x)$$

So we arrive at the time-independent Schrödinger's equation, substituting back in $E = \hbar\omega$:

$$E\psi(x) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) + V(x)\psi(x) \tag{11}$$

This gives us the founding equation of quantum mechanics, the culmination of all the experimental mysteries and inconsistencies found in the early twentieth century. Using this equation, we can find the wave function of a particle, which encapsulates all the information we require about its state and behaviour, dependent only on its energy and potential. It proved to be the key insight into the new world of quantum mechanics, and is therefore surprising in its simplicity and conciseness, compared to the complexity of the quantum world.

4.4 Interpretation of Schrödinger's Equation

Schrödinger's equation is the governing equation for motion in the smallest scale of magnitude. It links together energy, evolution in time, and evolution in space within the framework of quantum mechanics and its departures from the classical model. These differences with Newton's physics are immediately clear.

The $\Psi(x,t)$ term represents not a tangible physical quantity, but rather the *wave function*, which combines together waves with particles. We incorporated the fundamentals of wave-particle duality into our derivation, which has interesting physical implications, as what would classically be considered as a particle is treats based on wave-like properties like the de Broglie wavelength and frequency. The wave function is not even rooted in real numbers, but rather is some wave in the complex plane. Its physical significance lies in the fact that its modulus squared $|\psi\psi*|$ is a real number and represents the probability distribution of the particle[19]. This is how likely it is to be found at some given point in space and time. Rather than the ideal point particle of Newton's equations, the quantum particle contains inherent uncertainty of its position and momentum. Instead of occupying a point in space, it is rather distributed throughout space, with an associated probability of being at each point.

Usually, we use probabilities to quantify ignorance. If we know all equations of motion and the initial conditions, we can determine which side a coin will land on. However, when we do not know all these conditions, we have to resort to macroscopic probabilities. This is not the case here, as the wave function will 'collapse' to one of several possible states truly randomly, and will only follow the probabilistic distribution over a large number of observations. The wave function has all of these possible states as components[20], each scaled by how likely it is to occur. We say that the wave function is a *superposition* of these different states.

However, we cannot ever observe anything in two states at once[21]. Instead, when a measurement is taken, the wave function collapses instantly into one of its superimposed states[22]. Many prominent physicists at the time, including Einstein and Schrödinger himself, disliked this interpretation because it was so different to our intuitive vision of the world. After all, classically it is taken as axiomatic that one thing can never be in two places at once, and Schrödinger famously attempted to highlight the counter-intuitiveness of this interpretation with his thought experiment of a cat simultaneously dead and alive.

Einstein argued that there must be some *hidden variable* that determines the state of the wave function, however this was challenged in 1964 by the British physicist John Bell with his famous inequalities[23].

Despite the seemingly unintuitive picture of the world it presents, the equations of quantum mechanics work with extremely high accuracy to predict the results of experiments with atomic and subatomic particles. The field is still developing and changing, but quantum mechanics, and later quantum field theory, has proved to be the best model ever theorised to predict the behaviour on the smallest of scales.

5 Realisation and Results

Introduction

Once we had derived Schrödinger's equation, we decided to focus on understanding how it is used to solve quantum systems. We can use Schrödinger's equation to find the wave function and therefore probability distribution of a particle in certain situations. Since the idea of the wave function is often seen as abstract and unintuitive, we started with the most basic case of the infinite potential well to gain some understanding for what form the wave function could take. We then increased the complexity of our models, progressing onto finite potential wells and barriers. This allowed us to generate plots and graphs which helped us to better communicate the meaning behind the wave function and its probability distribution. These visualisations would help to highlight how the solutions to Schrödinger's equation differed in nature to the predictions made by classical physics.

5.1 Solution to Infinite Potential Well

Here we will consider the theoretical case where a particle is 'trapped' in a region between $x = 0$ and $x = a$ where there is zero potential energy, and outside of this region the potential energy is infinite. This means the particle can never leave this region.

The infinite potential well can be divided into three regions:

$$V(x) = \begin{cases} \infty & x < -L \\ 0 & -L \leq x \leq L \\ \infty & L < x \end{cases}$$

We will call the three regions Region I, II, III respectively.

Since the potential is infinite in Regions I and III, there is a zero probability of finding the particle there, so $\psi(x) = 0$ in these regions. However, in Region II, we can apply the time independent Schrödinger's equation (Equation [10]) to find $\psi(x)$:

$$E\psi(x) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) + V(x)\psi(x)$$

Since $V(x) = 0$ here,

$$\frac{\partial^2}{\partial x^2}\psi(x) = -\frac{2mE}{\hbar^2}\psi(x)$$

$$\frac{\partial^2}{\partial x^2}\psi(x) = -k^2\psi(x) \tag{12}$$

where $k^2 = \frac{2mE}{\hbar^2}$

Therefore we need an equation for the wave function where the second derivative is proportional to its negation. This property is seen in both sine and cosine so the function could take the form:

$$\psi(x) = A\cos(kx) + B\sin(kx) \tag{13}$$

We can check this to see it produces the desired second derivative.

$$\begin{aligned} \frac{d\psi}{dx} &= -kA\sin(kx) + kB\cos(kx) \\ \frac{d^2\psi}{dx^2} &= -k^2A\cos(kx) - k^2B\sin(kx) \\ &= -k^2\left[A\cos(kx) + B\sin(kx)\right] \\ &= -k^2\psi(x) \end{aligned}$$

At the boundaries $x = 0$ and $x = L$, the wave function should be continuous with the wave function outside the well. This tells us that it must equal 0 at these points

Solving the wave function at $x = 0$, we can see that:

$$\begin{aligned}\psi(0) = 0 &= A\cos(0) + B\sin(0)\\ &= A\\ \Rightarrow A &= 0\end{aligned}$$

Solving the wave function at $x = L$, we can see that:

$$\begin{aligned}\psi(L) = 0 &= A\cos(kL) + B\sin(kL))\\ &= B\sin(kL)\end{aligned}$$

So,

$$\begin{aligned}&\sin(kL) = 0\\ &\Rightarrow kL = n\pi \text{ , where } n \in \mathbb{N}\end{aligned}$$

This imposes quantisation on the system as, since L is constant, k can only take certain values corresponding to n. The case where $B = 0$ is also not considered as this would imply that $\psi(x) = 0$ at all points indicating that there is no wave.

Simplifying the wave function gives us:

$$\psi(x) = B_n \sin\left(\frac{nx\pi}{L}\right) \tag{14}$$

$$\begin{aligned}\text{where } k_n &= \frac{n\pi}{L}\\ \text{and } E_n &= \frac{n^2\hbar^2\pi^2}{2mL^2}\end{aligned}$$

The square of the wave function's amplitude represents the probability of a particle being present at that point. The sum of the probabilities across all these points should therefore be equal to 1. We can use this to find the value of B.

$$\begin{aligned}1 &= \int_0^L |\psi(x)|^2 dx\\ &= \int_0^L B^2 \sin^2\left(\frac{nx\pi}{L}\right) dx\\ &= \frac{B^2}{2}\int_0^L \cos^2\left(\frac{2nx\pi}{L}\right) dx\\ &= \frac{B^2}{2}\int_0^L \frac{1}{2}\left[1 - \cos\left(\frac{2nx\pi}{L}\right)\right] dx\\ &= \frac{B^2}{2}\left[x - \frac{L}{2n\pi}\sin\left(\frac{2nx\pi}{L}\right)\right]_{x=0}^{x=L}\\ &= \frac{B^2 L}{2}\\ B &= \sqrt{\frac{2}{L}}\end{aligned}$$

Substituting back into Equation [14], this gives us a final equation for the wave function of:

$$\psi(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{nx\pi}{L}\right) \tag{15}$$

When we take the square of the modulus of the wave function ($\psi\psi*$), this represents the probability distribution of the particle, showing how likely the particle is to be found at each point in space. The graphs below show the probability distributions for the particle in an infinite potential well in ascending energy levels n. The particle can only take these discrete levels, which are called stationary states, as the wave function will not evolve with time while the system remains the same. It should be noted that there are in fact a countably infinite number of these, and the first five are displayed below in Figure 2. This is a major departure from the classical model, which treats energy as taking any value in a continuous range. In general, when a particle is 'confined', its energy will be quantised, only allowed to take certain discrete values. This is often a value that must be solved for. A real world particle can exist in a superposition of many of these energy states, but will always collapse to one of them when an observation is made.

Energy levels of a particle in an infinite potential well

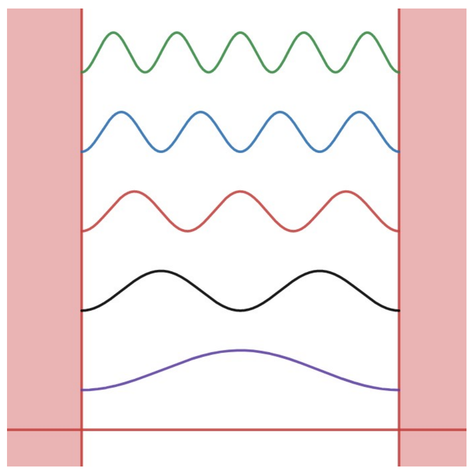

Figure 2: $\psi\psi*$ (probability distribution) at different energy levels n

We can see that as the energy of the particle increases, the wave function's wavelength decreases, and there are more areas of equal and maximum probability of the particle being found, were a measurement to be taken. Since the potential in this scenario is infinite, this can never occur in the physical world. However, this scenario has helped us gain some understanding of the nature and significance of the wave function.

5.2 Finite Potential Well

The infinite potential well is a non-physical theoretical situation. In the natural world, we see continuous, finite potentials, and we can therefore make our set up more realistic by studying a finite potential well. Here, the boundaries of the well are not infinitely strong, but can be overcome. This is analogous to a ball in a box: while the ball does not have sufficient energy to break through the box, it is confined to it. Classically, the ball could never leave the box, however the quantum particle has a non-negligible probability of being found within the walls of the potential well.

$$V(x) = \begin{cases} V_1 & x < 0 \\ 0 & 0 \leq x \leq L \\ V_2 & x > L \end{cases}$$

If the energy of the quantum particle within the well is less than the potential of the barriers, then it is in a 'bound state'. This means it can not escape the well, since it cannot overcome the barrier. Like in the infinite potential well, the bound states correspond to discrete energy levels, but in this case there are only a finite number of them. In this solution we will only consider bound cases where the energy of the particle E is less than V_1 and V_2. The unbound states will not be confined to the potential well and can escape, since they can overcome the walls of the well and become a travelling wave.

To solve this finite potential well to find ψ, we will have to apply Schrödinger's equation in each of the regions I, II, III. We will use the time independent equation from Equation [11], since this set up is static.

Region I: $x < 0$**,** $V(x) = V_1$

Using the time-independent Schrödinger's equation,

$$E\psi(x) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) + V_1\psi(x)$$

So

$$\begin{aligned}\frac{\partial^2}{\partial x^2}\psi(x) &= -\frac{2m(V_1 - E)}{\hbar^2}\psi(x) \\ &= k^2\psi(x) \text{ where } k = \frac{1}{\hbar}\sqrt{2m(V_1 - E)}\end{aligned}$$

This is a second order differential equation with a standard result that $\psi(x) = Ae^{-kx} + Be^{kx}$, where A and B are constants. We know that as $x \to -\infty$, $\psi(x) \to 0$, since the probability of finding a bound particle infinitely far from the well is zero. This also ensures that the wave function can be normalised. So $A = 0$, and $\psi(x) = Be^{kx}$ in Region I.

Region II: $0 \leq x \leq L$**,** $V(x) = 0$

$$E\psi(x) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x)$$

So

$$\begin{aligned}\frac{\partial^2}{\partial x^2}\psi(x) &= -\frac{2mE}{\hbar^2}\psi(x) \\ &= -q^2\psi(x) \text{ where } q = \frac{1}{\hbar}\sqrt{2mE}\end{aligned}$$

This is the same as Region II of the infinite potential well, and again gives us $\psi(x) = C\sin(qx) + D\cos(qx)$, where C and D are some constants.

Region III: $x > L$**,** $V(x) = V_2$

This can be solved in exactly the same way as Region I, and gives us $\psi(x) = Fe^{-\mu x}$, where F is some constant and $\mu = \frac{1}{\hbar}\sqrt{2m(V_2 - E)}$

$$\psi(x) = \begin{cases} Be^{kx} & x < 0 \\ C\sin(qx) + D\cos(qx) & 0 \leq x \leq L \\ Fe^{-\mu x} & x > L \end{cases}$$

This gives us 4 unknown constants (B, C, D, and F). However, we have 5 conditions, which are listed below. Conditions 1 and 3 require the wave function to be continuous at each boundary of the well, and conditions 2 and 4 require the gradient of the wave function to also be continuous at the boundaries. The final condition is the normalisation condition, requiring that the total probability of finding the particle in all space is 1. This is calculated as an integral of the probability distribution $\psi\psi*$ from $-\infty$ to ∞ in x.

1. $\psi_I(0) = \psi_{II}(0)$ (continuous at left hand boundary)

2. $\psi_I^{'}(0) = \psi_{II}^{'}(0)$ (gradient continuous at left hand boundary)

3. $\psi_{II}(L) = \psi_{III}(L)$ (continuous at right hand boundary)

4. $\psi_{II}^{'}(L) = \psi_{III}^{'}(L)$ (gradient continuous at right hand boundary)

5. $\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$ (normalisation condition)

We will use the conditions to rewrite all our constants in terms of B, and then normalise to find B.

The fifth unknown, which is required to balance the 5 conditions, is the energy of the particle. As mentioned earlier, since this particle is 'confined' in the well, the energy E can only take certain discrete energy levels, which we will need to solve for, since k, q, and μ depend on E.

Note

$$\psi'(x) = \begin{cases} kBe^{kx} & x < 0 \\ qC\cos(qx) - qD\sin(qx) & 0 \leq x \leq L \\ -\mu Fe^{-\mu x} & x > L \end{cases}$$

Condition 1: $\psi_I(0) = \psi_{II}(0)$

$$Be^0 = C\sin(0) + D\cos(0)$$

$$\rightarrow B = D \tag{16}$$

Condition 2: $\psi_I'(0) = \psi_{II}'(0)$

$$\begin{aligned} kBe^0 &= qC\cos(0) - qD\sin(0) \\ kB &= qC \end{aligned}$$

$$\rightarrow C = \frac{kB}{q} \tag{17}$$

Condition 3: $\psi_{II}(0) = \psi_{III}(0)$

$$Fe^{-\mu L} = C\sin(qL) + D\cos(qL)$$

From Equations [16] and [17], we can rewrite this as:

$$= B\left(\frac{k}{q}\sin(qL) + \cos(qL)\right)$$

$$\rightarrow F = Be^{\mu L}\left(\frac{k}{q}\sin(qL) + \cos(qL)\right) \tag{18}$$

Condition 4: $\psi_{II}'(0) = \psi_{III}'(0)$

$$-\mu Fe^{-\mu L} = qC\cos(qL) - qD\sin(qL)$$

Substituting in Equations [16], [17], and [18] allows us to eliminate C, D, and F by writing them in terms of B:

$$-\mu Be^{-\mu L}e^{\mu L}\left(\frac{k}{q}\sin(qL) + \cos(qL)\right) = qB\left(\frac{k}{q}\cos(qL) - \sin(qL)\right)$$

We can now remove B from our equation, leaving only terms that depend on E. We will normalise to find B later, and this will give us all the other constants.

$$-\mu\left(\frac{k}{q}\sin(qL) + \cos(qL)\right) = k\cos(qL) - q\sin(qL)$$

Dividing by $-\cos(qL)$ gives us

$$\begin{aligned} \frac{\mu k}{q}\tan(qL) + \mu &= q\tan(qL) - k \\ \left(q - \frac{\mu k}{q}\right)\tan(qL) &= \mu + k \\ \tan(qL) &= \frac{q\mu + qk}{q^2 - \mu k} \end{aligned}$$

Substituting $k = \frac{1}{\hbar}\sqrt{2m(V_1 - E)}$, $q = \frac{1}{\hbar}\sqrt{2mE}$, and $\mu = \frac{1}{\hbar}\sqrt{2m(V_2 - E)}$ back in:

$$\tan\left(\frac{L}{\hbar}\sqrt{2mE}\right) = \frac{\left(\frac{2m}{\hbar^2}\sqrt{EV_2 - E^2}\right) + \left(\frac{2m}{\hbar^2}\sqrt{EV_1 - E^2}\right)}{\left(\frac{2mE}{\hbar^2}\right) - \left(\frac{2m}{\hbar^2}\sqrt{E^2 - E(V_1 + V_2) + V_1V_2}\right)}$$
$$= \frac{\sqrt{EV_2 - E^2} + \sqrt{EV_1 - E^2}}{E - \sqrt{E^2 - E(V_1 + V_2) + V_1V_2}}$$

$$\tan\left(\frac{L}{\hbar}\sqrt{2mE}\right) = \frac{\sqrt{V_2 - E} + \sqrt{V_1 - E}}{\sqrt{E} - \sqrt{E - (V_1 + V_2) + \frac{V_1V_2}{E}}} \tag{19}$$

This equation is *transcendental*, meaning it cannot be solved analytically. We therefore have to resort to numerical methods to obtain solutions for z (and therefore for E). To do this, we used the Newton-Raphson method for numerically finding roots of functions. This is an iterative process of:

- Select a seed value of x
- Find the tangent to the function at that x
- The next value of x used is where this tangent intersects the x-axis
- so $x_{n+1} = x_n - \frac{f(x_n)}{f'(x_n)}$

This process gets closer and closer to the roots of functions, as shown in Figure 3[24] below.

Newton-Raphson method for numerical analysis

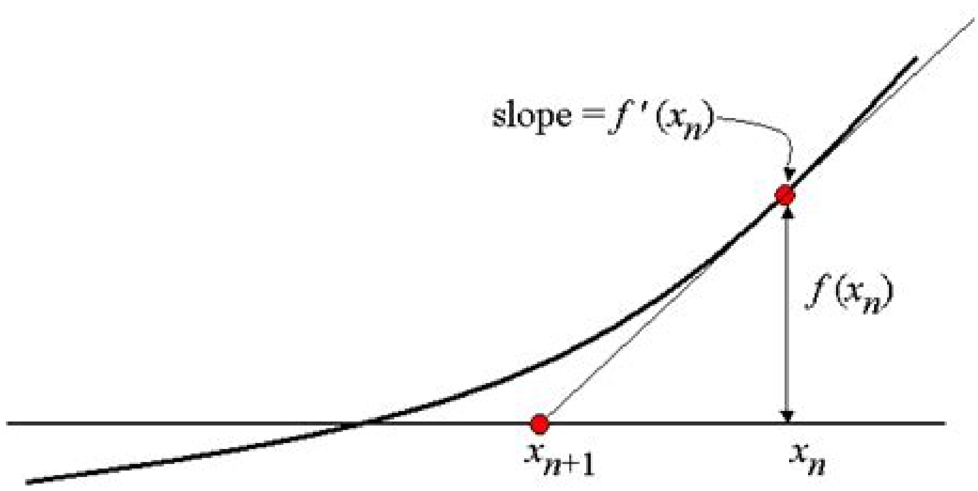

Figure 3: Newton-Raphson method for finding roots of functions

However, $\tan\left(\frac{L}{\hbar}\sqrt{2mE}\right)$ does not have a regular period, which makes selecting seed values for x very difficult. We will therefore change our equation to make the period of the tan function regular.

Let $z = \sqrt{E}$ and $a = \frac{L}{\hbar}\sqrt{2m}$. We have

$$tan(az) = \frac{\sqrt{V_2 - z^2} + \sqrt{V_1 - z^2}}{z - \sqrt{z^2 - (V_1 + V_2) + \frac{V_1V_2}{z^2}}} \tag{20}$$

Each solution to this equation represents an allowed bound energy level. Figure 4 below shows the solutions for a proton when $L = 2 \cdot 10^{-10}$m, $V_1 = 1.5$eV, $V_2 = 2$eV. The green line is the function $\tan(az)$, the red is the right hand side of Equation [20]. Each intersection is a solution.

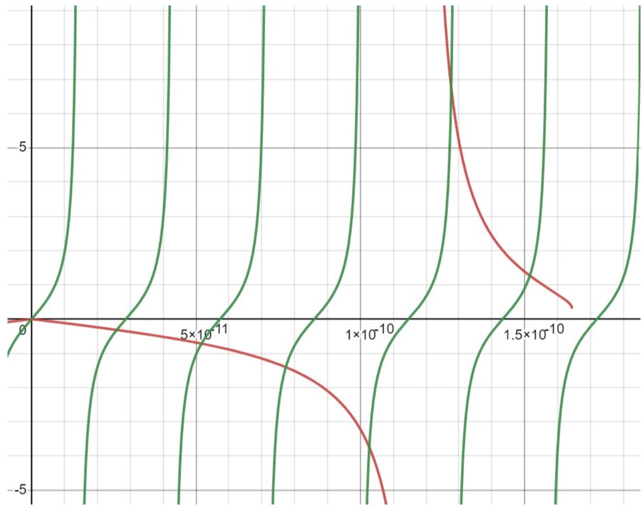

Figure 4: Graph representing allowed bound energy levels

The Newton-Raphson method is used to find roots of functions. In this case, we are finding roots of the function:

$$f(z) = \tan(az) - \frac{\sqrt{V_2 - z^2} + \sqrt{V_1 - z^2}}{z - \sqrt{z^2 - (V_1 + V_2) + \frac{V_1 V_2}{z^2}}}$$

$$f'(x) = a\sec^2(az) - \frac{-\frac{z}{\sqrt{V_2 - z^2}} - \frac{z}{\sqrt{V_1 - z^2}}}{z - \sqrt{z^2 + \frac{V_1 V_2}{z^2} - V_2 - V_1}} + \frac{\left(\sqrt{V_2 - z^2} + \sqrt{V_1 - z^2}\right)\left(1 - \frac{2z - \frac{2V_1 V_2}{z^3}}{2\sqrt{z^2 + \frac{V_1 V_2}{z^2} - V_2 - V_1}}\right)}{\left(z - \sqrt{z^2 + \frac{V_1 V_2}{z^2} - V_2 - V_1}\right)^2}$$

We choose seed values for x at each root of $\tan(az)$, which occur every $\frac{\pi}{a}$. To find the solutions around the asymptote of the red line in Figure 4, we first find the other solutions before and after the asymptote, and then choose seed values half way between the asymptote and the nearest root of $\tan(az)$ either side. If the solution we approach is the same as one we have already found, the next seed value will be half way between the previous seed value and the asymptote. This means the seed values get progressively closer to the asymptote until we approach the solutions just after and just before the asymptote. The code used to carry out this numerical solution can be found in Item 1 of the Appendix.

Once we have found z, we can then calculate E. This gives us k, q, and μ. We then only need to normalise to find B, which then gives us all the other constants, completely defining $\psi(x)$. For the normalisation of B, see Item 3 of the Appendix. This then allows us to plot the wave function and the probability distribution $\psi\psi*$, which represents the probability distribution of the quantum particle in the potential well. For the code used to plot these, see Item 1 of the Appendix.

In our graphs, since we divided our space into discrete regions in order to plot the wave function at regular intervals, we were able to check the normalisation was accurate by summing all $\psi\psi*$ with the width of each region of space. We found this was equal to 1 to several decimal places until the last energy level, at which point the wavelength was too short for this to be as accurate, and results were within 2% of 1.

5.3 Plots and Analysis

The Python program we wrote (found in Item 1 of the Appendix) solves the finite potential well, taking in V_1 and V_2, the mass of the particle m, and the width of the well L. The program performs the Newton-Raphson numerical solution on Equation [20] to find the allowed bound energy levels and therefore the wave function in each region. We then used the *matplotlib* Python library to plot the wave function and also the probability distribution, found by taking the square of the modulus of the wave function. For example, the graphs below are for a proton in the fourth energy level ($n = 4$) for a potential well of width $2 \cdot 10^{-10}$m and of potential 0.2eV on either side. The central region between the two black lines shows the behaviour inside the well, while the plots to the sides of these lines show the behaviour outside of the well.

Proton in symmetric potential well of 0.2eV

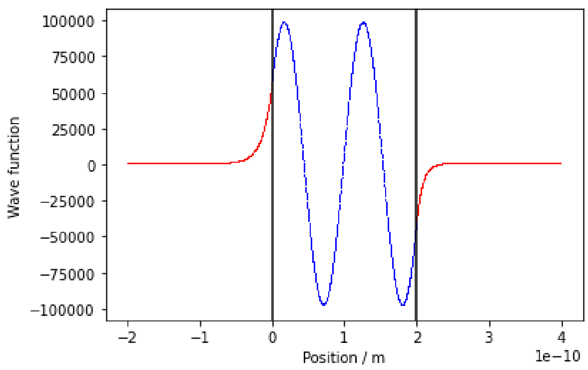

Figure 5: Wave function $\psi(x)$

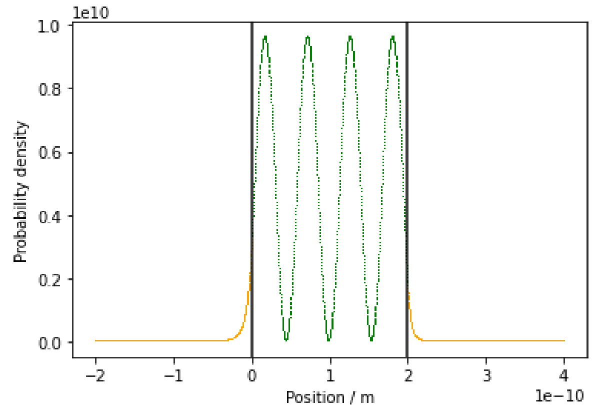

Figure 6: Probability distribution $(\psi\psi*)$

Within the well itself, the wave function is sinusoidal in nature, but exponentially decays in the regions of potential. This is seen in the probability distribution since the chance of finding the particle outside of the well is very small. A key point to note here is that the probability of finding the particle at different points within the well is not uniform, rather the probability distribution too takes a sinusoidal form. The number of peaks of this distribution, where the particle is most likely to be found when an observation is made, increases with the energy level, as shown below.

Probability distribution $\psi\psi*$ at increasing energy levels

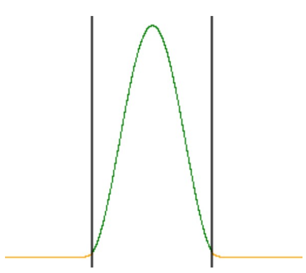

Figure 7: n = 1

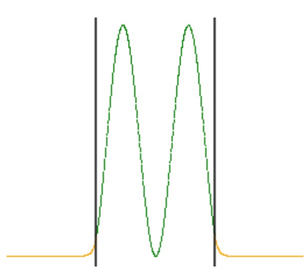

Figure 8: n = 2

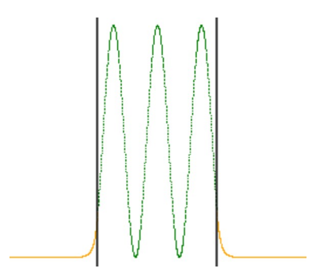

Figure 9: n = 3

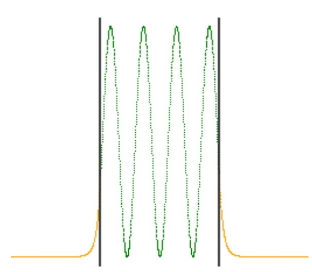

Figure 10: n = 4

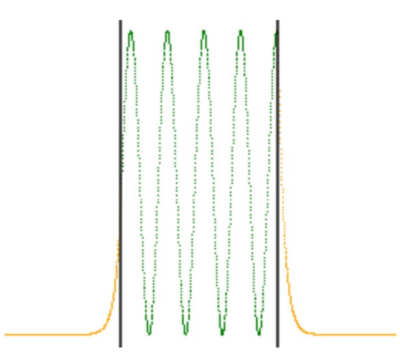

Figure 11: n = 5

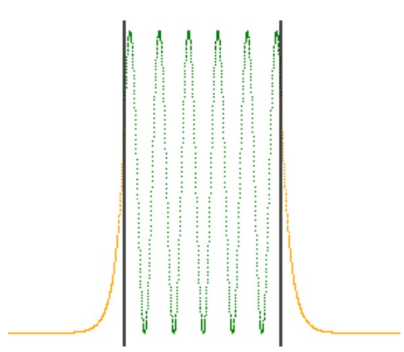

Figure 12: n = 6

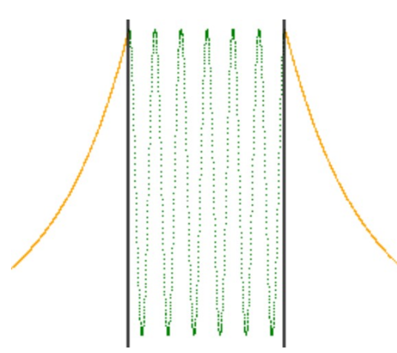

Figure 13: n = 7

The probability of the particle being outside of the well increases with the energy of the particle as well. Figure 13 at the seventh excited level shows the proton is in fact more likely to be found outside of the well than inside it, whereas in Figure 7 at the ground state, there is an almost zero probability of the particle leaving the well. This prompts the question of what would occur if another region of zero potential were to be placed on the other side of boundary of the well. It appears that the particles in high energy levels could move through the region of potential from the well to this region of zero potential. This does occur and is explored in detail in the *Finite Potential Barrier* section later.

These cases are symmetric, since $V_1 = V_2$, but when $V_2 > V_1$, the wave function will no longer be the same either side of the centre of the well. In this case, the bound solutions are only when $E < V_1 < V_2$. If the energy of the particle is greater than either of the two potentials, the particle will be able to escape the well, similar to how a ball can roll over a hill to the other side if it is moving fast enough. For example, Figure 14 below shows the bound energy levels for a proton when $V_1 = 0.2$eV and $V_2 = 0.4$eV, where the energy of the bound stationary states are in blue, and V_1 and V_2 are plotted in red.

Bound energy levels

Figure 14: The bound energy levels for $V_1 = 0.2$eV, $V_2 = 0.4$eV

When we plot the wave function for this non-symmetric set up, we see a bias towards the side of weaker potential, with the central peak of the sinusoidal central region shifted. In these graphs, $V_1 = 0.1$eV and $V_2 = 1.0$eV.

Wave function and probability distribution for a proton in a non-symmetric potential well

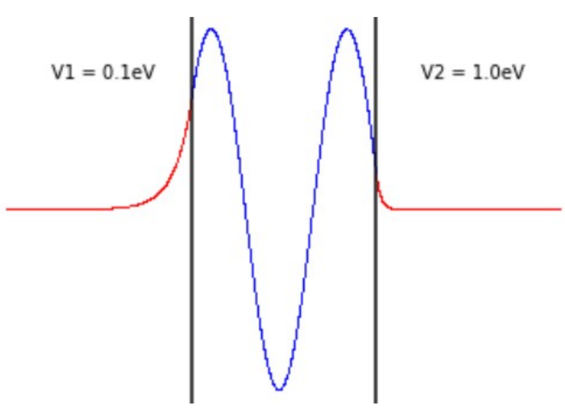

Figure 15: $\psi(x)$ when $V_1 = 0.1$eV, $V_2 = 1.0$eV

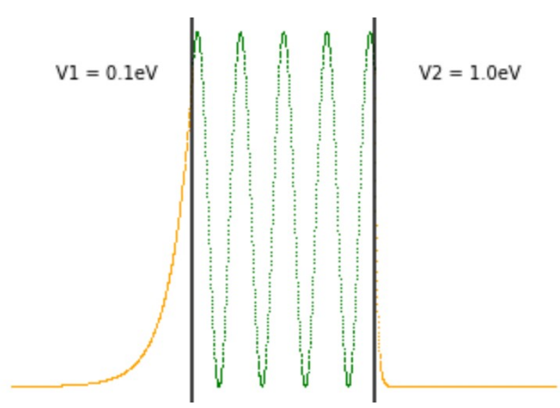

Figure 16: $\psi\psi*$ when $V_1 = 0.1$eV, $V_2 = 1.0$eV

Figure 16 shows how the particle is much more likely to move out of the well into the area of weak potential compared to the region of stronger potential. In the figure above, the potential to the right is ten times stronger than that on the left, so a much greater skew within the well might be expected. However, it is perhaps surprising to note the behaviour inside the well is very similar to that of a symmetric potential well, with only a slight shift towards the side of weaker potential.

These cases are important to consider since in real world scenarios, potentials are not ideal or symmetric. Most real world situations involve a smooth potential as a function of space and possibly also time, but these systems require much more computational power to simulate. Studying these simplifications help us to visualise the wave function, informing our understanding of how particles behave differently in quantum mechanics compared to classical physics. Just as idealised modelling assumptions in classical mechanics allows us to understand the behaviour of systems, potential wells serve as a foundation for modelling real world systems of greater complexity.

Specifically, this strictly theoretical idea of an ideal potential well can be applied to construct a model of the atom, describing the behaviour of electrons in it. These electrons can only occupy discrete energy levels, however altogether they form an 'electron cloud' which involves an uncertainty of where they exactly are at a given point in time. This quantum model differs from the classical one, in which electrons are considered as point particles instead of a probability distribution through space, which does not account for their quantum behaviour. This model is similar to a potential well, since electrons are 'trapped' in the atom, with an energy less than that required to escape. However, if the electrons are given enough energy, they can overcome this potential and escape the atom in the process known as *ionisation*. Potential wells are useful abstractions for these real world systems, but there are many other idealised scenarios that make the quantum behaviour observed in nature more accessible and easier to understand.

5.4 Finite Potential Barrier

One of the key differences of the quantum model to the classical model for the finite potential well was that the wave function is non-zero in the barrier, so the quantum particle can be found there. As mentioned earlier, it is therefore interesting to ask what the wave function would look like in the case where two potential wells are close together, so that the two wave functions of particles in each well overlap. To explore this, we will consider the finite potential barrier. This is a region of space with some potential, surrounded on both sides by regions of zero potential. A real world analogy would be a wall separating two empty rooms.

Classically, a particle approaching the barrier from one side could not travel to the other side, however in the quantum model, it can be shown that the particle can 'tunnel' through the barrier.

$$V(x) = \begin{cases} 0 & x < 0 \\ V_0 & 0 \leq x \leq L \\ 0 & x > L \end{cases}$$

Again we will assign the names Region I, II, III to each case respectively. We will only consider the cases where $E < V_0$ as these are the cases where the classical model forbids particles moving from one side of the barrier to the other.

Region I: $V(x) = 0$

From the time independent Schrödinger's equation,

$$E\psi(x) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x)$$

So

$$\begin{aligned} \frac{\partial^2}{\partial x^2}\psi(x) &= -\frac{2mE}{\hbar^2}\psi(x) \\ &= -k^2\psi(x) \text{ where } k = \frac{1}{\hbar}\sqrt{2mE} \end{aligned}$$

Here, we could represent $\psi(x)$ in terms of $\sin(kx)$ and $\cos(kx)$ as is done above. However, we will choose instead to use the alternative complex form of

$$\psi(x) = Ae^{ikx} + Be^{-ikx} \tag{21}$$

since the Ae^{ikx} term represents the approaching wave moving in the positive direction since the phase of the wave is increasing with x and the Be^{-ikx} term represents the part of the wave that is reflected at the border with the barrier. We choose this form because $|e^{ikx}| = 1$ for all x, so A is the modulus of the wave function. We will compare this to the modulus of the wave function on the other side of the barrier to find the probability of transmission.

Region II: $V(x) = V_0$ From the time independent Schrödinger's equation,

$$E\psi(x) = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi(x) + V_0\psi(x)$$

So

$$\begin{aligned} \frac{\partial^2}{\partial x^2}\psi(x) &= -\frac{2m(V_0 - E)}{\hbar^2}\psi(x) \\ &= q^2\psi(x) \text{ where } q = \frac{1}{\hbar}\sqrt{2m(V_0 - E)} \end{aligned}$$

Using the standard results from earlier,

$$\psi(x) = Ce^{qx} + De^{-qx} \tag{22}$$

Region III: $V(x) = 0$

This is the same as region I, and $\psi(x) = Fe^{ikx} + Ge^{-ikx}$. However, we will only consider the Fe^{ikx} term, since we are assuming there are no waves moving in the negative direction on the opposite side of the barrier. The transmitted wave will not be travelling back towards the barrier. So

$$\psi(x) = Fe^{ikx} \tag{23}$$

Since the approaching wave is a travelling wave, it extends back to $-\infty$, and the transmitted wave extends to ∞ in the positive direction. This wave function can therefore not be normalised, so we will have four boundary conditions for five constants (A, B, C, D, and F). We will therefore write A in terms of F, which will allow us to compare the two to find the probability of transmission through the barrier. Our conditions are the same as the four boundary conditions in the solution above for the finite potential well. It is important to note here that, since the particle is not 'confined' in the finite potential barrier set up, the energy of the particle is not restricted to discrete energy levels, but rather can take any value in a continuous range. E is therefore not a value that we need to find, but is instead a variable that we choose. In real world situations, though, the wave would not extend to ∞, but would be bounded by potentials somewhere on either side of the barrier. Irrespective of how far these regions of potential are from our potential barrier, this will 'confine' the particle and therefore enforce discrete, quantised energy levels. We have:

$$\psi(x) = \begin{cases} Ae^{ikx} + Be^{-ikx} & x < 0 \\ Ce^{qx} + De^{-qk} & 0 \leq x \leq L \\ Fe^{ikx} & x > L \end{cases}$$

And

$$\psi^{'}(x) = \begin{cases} ikAe^{ikx} - ikBe^{-ikx} & x < 0 \\ qCe^{qx} - qDe^{-qk} & 0 \leq x \leq L \\ ikFe^{ikx} & x > L \end{cases}$$

Condition 1: $\psi_I(0) = \psi_{II}(0)$ This condition gives us

$$Ae^0 + Be^0 = Ce^0 + De^0$$

So

$$A + B = C + D \tag{24}$$

Condition 2: $\psi_I^{'}(0) = \psi_{II}^{'}(0)$

We have

$$ikA - ikB = qC - qD \tag{25}$$

Multiplying Equation [24] by ik and adding it to Equation [25] gives us

$$2ikA = (ik + q)C + (ik - q)D$$

So

$$A = \frac{1}{2}\left(1 + \frac{q}{ik}\right)C + \frac{1}{2}\left(1 - \frac{q}{ik}\right)D \tag{26}$$

Condition 3: $\psi_{II}(L) = \psi_{III}(L)$

This condition gives us

$$Ce^{qL} + De^{-qL} = Fe^{ikL} \tag{27}$$

Condition 4: $\psi'_{II}(L) = \psi'_{III}(L)$

Here, we have

$$qCe^{qL} - qDe^{-qL} = ikFe^{ikL} \tag{28}$$

Multiplying Equation [27] by q gives

$$qCe^{qL} + qDe^{-qL} = qFe^{ikL} \tag{29}$$

Equation [28] added to Equation [29] leaves us with

$$2qCe^{qL} = (ik + q)Fe^{ikL-qL}$$

$$C = \frac{1}{2}\left(1 + \frac{ik}{q}\right)Fe^{ikL-qL} \tag{30}$$

Equation [81] taken away from Equation [82] similarly gives us

$$D = \frac{1}{2}\left(1 - \frac{ik}{q}\right)Fe^{ikL+qL} \tag{31}$$

Substituting these results back into Equation [26] gives

$$\begin{aligned} A &= \frac{1}{2}\left(1 + \frac{q}{ik}\right)\left[\frac{1}{2}\left(1 + \frac{ik}{q}\right)Fe^{ikL-qL}\right] + \frac{1}{2}\left(1 - \frac{q}{ik}\right)\left[\frac{1}{2}\left(1 - \frac{ik}{q}\right)Fe^{ikL+qL}\right] \\ &= \frac{1}{4}Fe^{ikl-qL}\left[\left(1 + \frac{q}{ik}\right)\left(1 + \frac{ik}{q}\right) + \left(1 - \frac{q}{ik}\right)\left(1 - \frac{ik}{q}\right)e^{2qL}\right] \\ &= \frac{Fe^{ikl-qL}}{4ikq}\left[(ik+q)^2 - (ik-q)^2e^{2qL}\right] \end{aligned}$$

This gives us the the relationship between A and F we were trying to find:

$$\frac{F}{A} = \frac{4ikqe^{qL-ikL}}{(ik+q)^2 - (ik-q)^2e^{2qL}} \tag{32}$$

Since the wave function in the finite potential barrier cannot be normalised, we can set $A = 1$. This allows us to generate all the other constants and we were therefore able to plot the wave function in the three different regions. While the classical model does not allow the particle to pass through the barrier, in the plots for the quantum particle, we see that the particle has a significant probability of tunneling through the barrier.

5.5 Plots and Analysis

In the above solution to the finite potential barrier, we arrived at a complex wave function, so we plotted the real and imaginary parts of $\psi(x)$ separately. The plots in Figures 17 − 25 below show the wave function of an electron with different energies as it approaches a 10eV potential barrier roughly the width of an atom (10^{-10}m) from the left. Classical physics would predict all of the wave to be reflected at the boundary with the barrier, with a zero probability of transmission, however we can see the quantum particle has some probability of tunneling through the barrier.

Real part of wave function $\Re(\psi(x))$

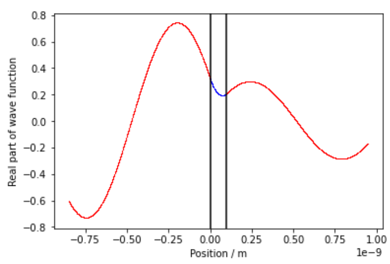

Figure 17: E = 2eV

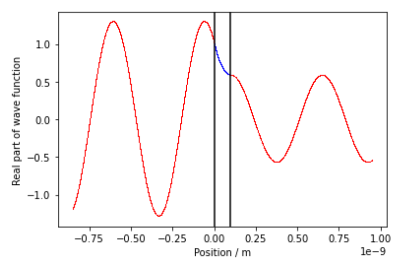

Figure 18: E = 5eV

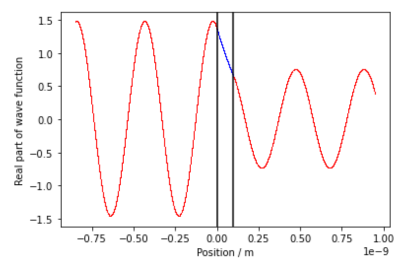

Figure 19: E = 9eV

Imaginary part of wave function $\Im(\psi(x))$

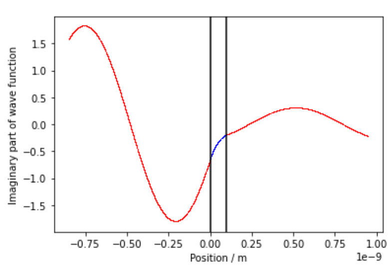

Figure 20: E = 2eV

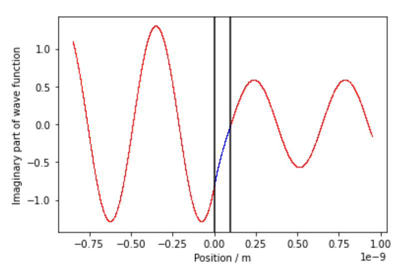

Figure 21: E = 5eV

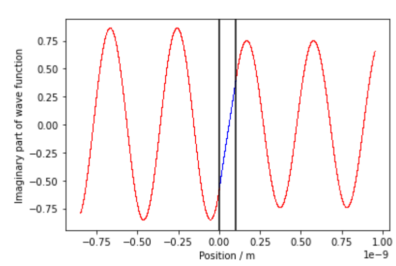

Figure 22: E = 9eV

Probability distribution $\psi\psi*$

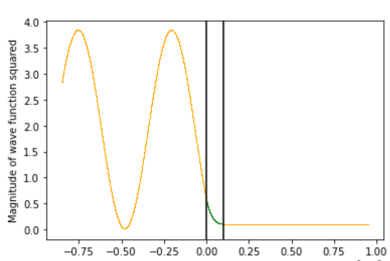

Figure 23: E = 2eV

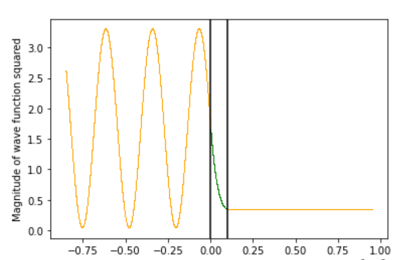

Figure 24: E = 5eV

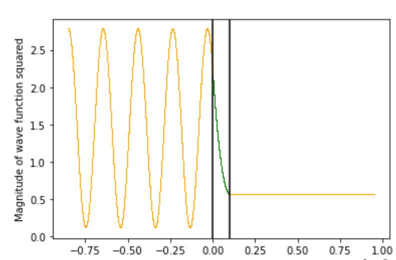

Figure 25: E = 9eV

The majority of the time, the electron will reflect at the barrier, but from Figures 23 − 25, we can see that the approaching electron has a significant chance of tunneling through the potential barrier and being found on the opposite side, since the value of $\psi\psi*$ is non-negligible in the rightmost region. It is worth noting here the implications of this effect, and how strongly it contradicts classical physics. If a ball is rolled up a hill with insufficient energy to reach the top, all of our intuition would lead us to believe that the ball must roll back down, and the notion that the ball could pass through to the opposite side of the hill seems an impossibility. Quantum tunneling removes any certainty that a particle trapped in a region from which it has insufficient energy to escape will remain there. More implications and examples of tunneling will be explored in the *Quantum tunneling in the real world* section.

By comparing the probability distribution for the electron with 2eV and 9eV in Figures 23 and 25, the chance of transmission clearly increases as the energy of the electron increases. We can in fact derive an expression for this probability of tunneling.

5.6 Probability of tunneling

As mentioned above, since $|e^{ikx}| = 1$ for all x, $\left|\frac{F}{A}\right|^2$ represents the ratio between the probability of finding the particle approaching the barrier in Region I and the probability of finding the particle having been transmitted T. This shows the probability of an approaching particle tunneling through the barrier.

From Equation [32], we have

$$\frac{F}{A} = \frac{4ikqe^{qL-ikL}}{(ik+q)^2 - (ik-q)^2 e^{2qL}}$$

So

$$\begin{aligned} T &= \left|\frac{F}{A}\right|^2 = \left(\frac{F}{A}\right)\left(\frac{F}{A}\right)^* \\ &= \left(\frac{4ikqe^{qL-ikL}}{(ik+q)^2 - (ik-q)^2 e^{2qL}}\right)\left(\frac{-4ikqe^{qL+ikL}}{(q-ik)^2 - (ik+q)^2 e^{2qL}}\right) \end{aligned}$$

By reintroducing our definitions for k and q and also using the hyperbolic trigonometric function:

$$\sinh(x) := \frac{e^x - e^{-x}}{2}$$

this can be simplified to

$$T = \frac{1}{1 + \frac{V_0^2 \sinh^2(qL)}{4E(V_0 - E)}} \tag{33}$$

For the complete working to arrive at this equation, see Item 4 of the Appendix.

Figure 26 below shows how the probability of an electron tunneling through a 10eV barrier changes at different energies and for different widths of barrier L.

The probability of tunneling at varying energies

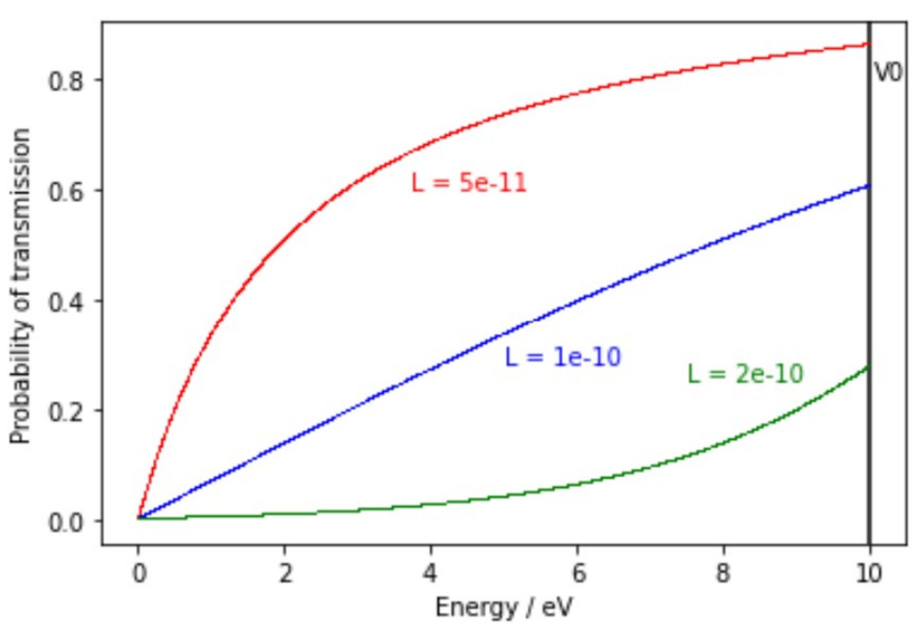

Figure 26: Probability of an electron tunneling through a 10eV barrier at varying energies for $L = 0.5 \cdot 10^{-10}$m (red), $L = 1.0 \cdot 10^{-10}$m (blue), and $L = 2.0 \cdot 10^{-10}$m (green)

From Figure 26, we see that while the energy of a particle is low relative the potential barrier, and while the barrier is wide, there is a low probability of transmission. However, as the barrier becomes thinner and the particle gains energy, the probability of transmission quickly increases. There are many physical systems with strong potential barriers that would be impossible to pass through according to classical equations, but the vast number of particles involved outweighs the small probability of tunneling. This means quantum tunneling can have a significant effect on the behaviour of the systems.

5.7 Quantum tunneling in the real world

Such a case is the process of fusion in the Sun, where two protons fuse together into a helium nucleus, releasing energy that prevents the Sun collapsing under gravity. However, for this to occur, the two protons must get close enough to interact via the strong force, which has a very short range (approximately $3 \cdot 10^{-18}$m). Therefore, they must have enough kinetic energy to overcome the electrostatic force of repulsion between them called the Coulomb barrier[25]. However, the thermal energy of the Sun is approximately 200 times less than that required to bring two protons close enough to go through nuclear fusion[26]. So classically this fusion should not be able to occur, and yet we observe it. As the protons approach the Coulomb barrier, there is a small chance of them tunneling through it into the region of strong force attraction. The Coulomb barrier is strong and also relatively wide, so the probability of transmission through it is small, however the vast number of protons in the Sun means that these fusions happen frequently. When the probability of transmission and the expended rate of fusion is calculated, the results match the amount of fusion happening in the Sun.

Similar tunneling occurs in many chemical reactions where the activation energy is greater than the energy of the reactants. One of the most fundamental reactions carried out by enzymes involves the transfer of hydrogen, but many of these reactions involve substrates with a large bond dissociation energy[27], which represents the energy required to break the existing bonds to enable a reaction to take place, hence there are large inherent barriers for the reaction. We observe this reaction at temperatures that are too low for the particles to have sufficient energy to overcome this bond dissociation energy. Again, the hydrogen may tunnel through this barrier to react with one another and serves as more evidence for tunneling in nature.

Understanding the behaviour of subatomic particles has enabled many of the advancements in modern computing, which revolves around manipulating electrons with astounding precision, and quantum mechanics has allowed electrical engineers to develop technologies on progressively smaller scales. As nanotechnology develops and the size of electrical components gets closer to the scales of molecules, though, quantum tunneling becomes a significant issue. For example, transistors, which are now being produced on scales of several nanometers[28], have started to be seriously affected by quantum tunneling.Transistors act as electrical switches, and therefore have barriers that prevent the flow of electrons when the transistor is switched off. As the barriers become thinner, the electrons have a greater chance of tunneling through them, significantly reducing the effectiveness of the transistor. This imposes a fundamental limit on the size of transistors[28], and is thought to be a major obstacle for future technological advancements. However, quantum computing[29] may serve as a solution to this problem, as it utilises such quantum effects, rather than being hindered by them. As physicists build their understanding of atomic scales, they become more able to manipulate these systems and build technologies that are not only capable of managing quantum effects like tunneling, but can in fact exploit these phenomena just as is often seen in the natural world.

5.8 Evaluation of our results

In the beginning of the project, we aimed to concisely cover the evolution of quantum mechanics, emphasising the key discoveries and deviations from the classical model. We felt this research was effective and allowed us to bridge many of the gaps in understanding preventing us from interpreting Schrödinger's equation. We found that researching the origins and complex ideas embedded into the equation helped us understand its meaning and significance when we replicated its derivation. Once this conceptual foundation was established, we were able to delve into Schrödinger's equation and its applications, and further analyse the quantum models mentioned in the brief. These models provided us with insights into quantum effects and the surprising behaviour of particles on subatomic scales. We prioritised creating visualisations for what are often difficult to grasp concepts. The Python programs we wrote to solve and plot solutions to our models helped to effectively communicate the physical significance of the wave function, as well as grasp the form that the probability distribution of particles takes in different quantum systems.

However, as mentioned earlier the systems we studied are relatively simple, and while they give useful insight into the nature of the wave function and the interpretation of particles in quantum mechanics, they are abstracted from the real-world systems we see in nature. Our solutions, for example, only consider one dimension, and we would have liked to expand our research to two and three dimensional set ups were we to continue our project further. Furthermore, an aspect of the brief that we would have liked to explore further is extending our models to more complex structures like a hydrogenic atom, building on our research into Bohr's model of the atom. Producing numerical simulations for these would have complimented our investigation into quantum models and reinforced our understanding of the wave function's significance in real-world systems. Throughout our project, we attempted to solve our models as analytically as possible by solving Schrödinger's equation as fully as we could before resorting to numerical analysis. Retrospectively, a useful methodology might have been to rely more heavily on numerical analysis, as this would have enabled us to adapt our programs more easily to the more complex set ups we would have liked to have explored.

Ultimately, though, we feel that we have covered all the main ideas that our project brief suggested. We have extensively explored how quantum mechanics diverges from classical physics, and built a detailed understanding of the Schrödinger equation and how it can be used.

Aside from gaining a deep understanding of this field of physics, we believe this project has benefited our communication and organisation skills, as well as improving our mathematical maturity. Working in a group of people, with distinct skills and opinions, yet all focused on a collaborative project has been a useful learning experience for all of us. Creating such an extensive piece of work over a long period of time has allowed us to experience the essence of research and academic writing, preparing us for future works.

6 Conclusion

In this paper, we have aimed to clearly explain some of the major departures from classical physics that arise in quantum mechanics. The solutions we found to Schrödinger's equation show how different behaviour is on subatomic scales to that which we intuitively recognise and understand. Even the basic representation of a particle in quantum models defies all classical notions, intertwining waves and particles together into one abstract function that does not even reside in the plane of real numbers. As the scale we are inquiring into becomes small enough, quantum behaviours take observable effect: pursuing certainty of position, momentum, and energy becomes inherently futile. Probabilities no longer encapsulate ignorance but rather fundamental randomness innate to quantum systems, with probability distributions for a particle able to seep into regions of space that are classically impossible for the particle to be found in.

Throughout this project quantum mechanics has proved to be an unintuitive, and hence intriguing field of physics. Its departure from the classical model has revolutionised our understanding of many observed physical phenomena. However, this breakthrough has not progressed without issues. We have repeatedly highlighted the many differences between the quantum mechanics from the classical model, but a more problematic discovery has been that quantum mechanics and Einstein's theory of relativity cannot coexist. Both of these fields work with astounding accuracy in their respective areas, the quantum models in the smallest observable objects and Einstein's relativity with large celestial bodies. However when attempted to be brought together both fail. This incompatibility has caused a major inconsistency in physics and has motivated many new ideas like 'String Theory'. Finding a hypothetical 'Theory of Everything' that unifies quantum mechanics and Einstein's relativity is still the main goal for the scientific community today, and many have deemed this search hopeless.

7 Appendix

Note all code in this appendix is written using Python 3.8

7.1 Code to plot solutions to a non-symmetric potential well

```
import math
from scipy.constants import hbar
import matplotlib.pyplot as plt

PI = math.pi
e = math.e
TRIES = 1000
SF_PRECISION = 10
STABILISE_REPEATS = 15
NO_OF_STEPS = 1000 #Number of plots inside the well

V1 = 1.6*10**-20 #LHS potential
V2 = 16*10**-20 #RHS potential
L = 2*10**-10 #Width of the potential well
m = 1.67 * 10**-27
a = (L/hbar) * math.sqrt(2*m)

STEP = L / NO_OF_STEPS

if V1 < V2:
    smaller = 'V1'
else:
    smaller = 'V2'

max_z = math.sqrt(min([V1, V2]))
Asymptote = math.sqrt((V1 * V2) / (V1 + V2))
Period = PI / a

def sf(x, SF):
    i = 0
    while str(x)[i] == '0':
      i += 1
    return str(x)[:SF + i + 1]

def round_solution(solution, SF_PRECISION):
    significant_digits = sf(solution, SF_PRECISION)
    mult = 0
    for i in range(len(str(solution))):
        if str(solution)[i] == 'e':
            mult = int(str(solution)[i+1:])
    return float(significant_digits) * (10**mult)
#FUNCTION TO NUMERICALLY SOLVE
def f(z, check = 0):
    zs = z**2
    if check == 'V1':
        zs = V1
    elif check == 'V2':
        zs = V2
    LHS = math.tan(a*z)
    RHS = math.sqrt(V1 - zs) + math.sqrt(V2 - zs)
    RHS /= z - math.sqrt(z**2 - (V1+V2) + ((V1*V2)/zs))
    return LHS - RHS
```

```python
#DERIVATIVE OF FUNCTION
def f_prime(z):
    S = math.sqrt(z**2 - (V1+V2) + ((V1*V2)/(z**2)))
    sec = 1/math.cos(a*z)
    term1 = (a*sec**2)
    term2 = z/math.sqrt(V1 - z**2) + z/math.sqrt(V2 - z**2)
    term2 /= z - S
    term3 = math.sqrt(V1 - z**2) + math.sqrt(V2 - z**2)
    term3 *= 1 - ((z - (V1*V2)/(z**3)) / S)
    term4 = (z - S) ** 2
    return term1 + term2 + (term3 / term4)

def Newton_Raphson(start):
    count = 0
    OK = False
    solution = -1
    prev_x = -1
    x_n = start
    rounded_solution = -1
    for cycle in range(TRIES):
        while x_n > max_z:
            x_n = 0.5 * (x_n + prev_x)
        f_x = f(x_n)
        fp_x = f_prime(x_n)
        x_n = x_n - (f_x / fp_x)
        if sf(x_n, SF_PRECISION) == sf(prev_x, SF_PRECISION):
            count += 1
        else:
            count = 0
            prev_x = x_n
        if count > STABILISE_REPEATS:
            solution = x_n
            rounded_solution = round_solution(solution, SF_PRECISION)
            OK = True
            break
    return OK, rounded_solution

def normalise_to_find_B(k, l, u):
    term1 = 1/(2*k)
    term2 = (l**2 - k**2) * math.sin(2*l*L)
    term2 -= 4*l*L * (math.cos(l*L))**2
    term2 += 2*L * l**3
    term2 += 2*l*L * k**2
    term2 += 4*k*L
    term2 /= 4 * l**3
    term3 = (math.cos(l*L) + (k/l) * math.sin(l*L)) ** 2
    term3 /= 2*u
    B = 1 / math.sqrt(term1 + term2 + term3)
    return B
#FIND NUMBER OF SOLUTIONS
number_below_asymptote = round(Asymptote / Period)
number_above_asymptote = round(max_z / Period) - round(Asymptote / Period)
if f(max_z, check = smaller) > 0:
    number_above_asymptote += 1
number_of_solutions = number_below_asymptote + number_above_asymptote
solutions = ()

#BEFORE ASYMPTOTE
start = 0
for n in range(number_below_asymptote - 1):
```

```
    start += Period
    OK, solution = Newton_Raphson(start)
    while not OK:
        start *= 1.01
        OK, solution = Newton_Raphson(start)
    solutions += (solution,)

#JUST BEFORE ASYMPTOTE
prev_tan_root = start
start = 0.5 * (prev_tan_root + Asymptote)
OK = False
while not OK:
    OK, solution = Newton_Raphson(start)
    if solution in solutions:
        OK = False
    start = 0.5 * (start + Asymptote)
solutions += (solution,)

#JUST AFTER ASYMPTOTE
next_tan_root = prev_tan_root + Period
start = 0.5*(next_tan_root + Asymptote)
OK = False
while not OK:
    OK, solution = Newton_Raphson(start)
    if solution in solutions:
        OK = False
    start = 0.5 * (start + Asymptote)
solutions += (solution,)

#AFTER ASYMPTOTE
start = next_tan_root
for n in range(number_above_asymptote - 1):
    start += Period
    OK, solution = Newton_Raphson(start)
    while not OK:
        start *= 1.01
        OK, solution = Newton_Raphson(start)
    solutions += (solution,)
energy_levels = [x**2 for x in solutions]
#SET UP PLOTS
plt.figure(0)
for n in range(number_of_solutions):
    E = energy_levels[n]
    ax1 = plt.axes(frameon=False)
    ax1.axes.get_xaxis().set_visible(False)
    plt.axhline(y=E, xmin=0, xmax=1, color = 'b')
    plt.plot(1, E, marker = ',', color='b')
    plt.text(1.06, E, f'n = {n+1}')

plt.axhline(y=V1, xmin=0, xmax=1, color = 'r')
plt.plot(1, V1, marker = ',', color='r')
plt.text(1.06, V1, 'V1')
plt.axhline(y=V2, xmin=0, xmax=1, color = 'r')
plt.plot(1, V2, marker = ',', color='r')
plt.text(1.06, V2, 'V2')
#SOLVE EACH ENERGY LEVEL
for n in range(number_of_solutions):
    max_phi = 0
    record_x = 0
    E = energy_levels[n]
```

```
k = (1/hbar) * math.sqrt(2*m*(V1-E))
l = (1/hbar) * math.sqrt(2*m*E)
u = (1/hbar) * math.sqrt(2*m*(V2-E))
B = normalise_to_find_B(k, l, u)
normalisation_sum_check = 0
#REGION 1
x = -L
while x < 0:
    phi = B * (e ** (k * x))
    plt.figure(2*n + 1)
    plt.plot(x, phi, marker = ',', color = 'r')
    plt.figure(2*n + 2)
    plt.plot(x, phi**2, marker = ',', color = 'orange')
    normalisation_sum_check += STEP * phi**2
    x += STEP
#REGION 2
while x < L:
    phi = B * (math.cos(l*x) + (k/l) * math.sin(l*x))
    plt.figure(2*n + 1)
    plt.plot(x, phi, marker = ',', color = 'b')
    plt.figure(2*n + 2)
    plt.plot(x, phi**2, marker = ',', color = 'g')
    normalisation_sum_check += STEP * phi**2
    x += STEP
    if n == 0:
        if phi > max_phi:
            max_phi = phi
            record_x = x
#REGION 3
while x < 2*L:
    phi = B * (math.cos(l*L) + (k/l) * math.sin(l*L)) * e**(u*(L-x))
    plt.figure(2*n + 1)
    plt.plot(x, phi, marker = ',', color = 'r')
    plt.figure(2*n + 2)
    plt.plot(x, phi**2, marker = ',', color = 'orange')
    normalisation_sum_check += STEP * phi**2
    x += STEP
#PLOT DETAILS
plt.figure(2*n + 1)
plt.axvline(x=0, color = 'black')
plt.axvline(x=L, color = 'black')
plt.xlabel('Position / m')
plt.ylabel('Wave function')
plt.text(-0.75*L, 0.75*max_phi, f'V1 = {V1}', color = 'black')
plt.text(1.25*L, 0.75*max_phi, f'V2 = {V2}', color = 'black')
plt.figure(2*n + 2)
plt.axvline(x=0, color = 'black')
plt.axvline(x=L, color = 'black')
plt.xlabel('Position / m')
plt.ylabel('Probility density')
plt.text(-0.75*L, 0.75*max_phi**2, f'V1 = {V1}', color = 'black')
plt.text(1.25*L, 0.75*max_phi**2, f'V2 = {V2}', color = 'black')
```

7.2 Code to plot solutions to a finite potential barrier

```
import math
from scipy.constants import hbar
import matplotlib.pyplot as plt

PI = math.pi
e = math.e
i = 1j

L = 10**-10 #Width of barrier
V0 = 16*10**-19 #Potential of barrier
m = 9.11*10**-31 #mass of quantum particle

NO_OF_STEPS = 500 #Number of plots inside the barrier
rel_width = 1/18 #Relative width of the barrier on the plot
STEP = L / NO_OF_STEPS

E = 2*10**-19 #Energy of quantum particle
A = 1 #Set A as 1 as this is arbitrary

#CALCULATE CONSTANTS
k = 1/hbar * math.sqrt(2*m*E)
q = 1/hbar * math.sqrt(2*m*(V0-E))
F = A * 4*i*k*q*e**(q*L - i*k*L)
F /= (q + i*k)**2 - (e**(2*q*L))*((q-i*k)**2)
C = 0.5 * (1 + i*k/q) * e**(i*k*L-q*L) * F
D = 0.5 * (1 - i*k/q) * e**(i*k*L+q*L) * F
B = C + D - A

#REGION 1
minx = -(((1/rel_width) - 1) / 2) * L
x = minx
while x < 0:
    phi = A*e**(i*k*x) + B*e**(-i*k*x)
    real_phi = phi.real
    imag_phi = phi.imag
    phi_sq = real_phi**2 + imag_phi**2
    plt.figure(1)
    plt.plot(x, real_phi, marker = ',', color = 'r')
    plt.figure(2)
    plt.plot(x, imag_phi, marker = ',', color = 'r')
    plt.figure(3)
    plt.plot(x, phi_sq, marker = ',', color = 'orange')
    x += STEP
#REGION 2
while x < L:
    phi = C*e**(q*x) + D*e**(-q*x)
    real_phi = phi.real
    imag_phi = phi.imag
    phi_sq = real_phi**2 + imag_phi**2
    plt.figure(1)
    plt.plot(x, real_phi, marker = ',', color = 'b')
    plt.figure(2)
    plt.plot(x, imag_phi, marker = ',', color = 'b')
    plt.figure(3)
    plt.plot(x, phi_sq, marker = ',', color = 'green')
    x += STEP
#REGION 3
while x < L - minx:
```

```
    phi = F*e**(i*k*x)
    real_phi = phi.real
    imag_phi = phi.imag
    phi_sq = real_phi**2 + imag_phi**2
    plt.figure(1)
    plt.plot(x, real_phi, marker = ',', color = 'r')
    plt.figure(2)
    plt.plot(x, imag_phi, marker = ',', color = 'r')
    plt.figure(3)
    plt.plot(x, phi_sq, marker = ',', color = 'orange')
    x += STEP
#PLOT DETAILS
plt.figure(1)
plt.axvline(x=0, color = 'black')
plt.axvline(x=L, color = 'black')
plt.xlabel('Position / m')
plt.ylabel('Real part of wave function')
plt.figure(2)
plt.axvline(x=0, color = 'black')
plt.axvline(x=L, color = 'black')
plt.xlabel('Position / m')
plt.ylabel('Imaginary part of wave function')
plt.figure(3)
plt.axvline(x=0, color = 'black')
plt.axvline(x=L, color = 'black')
plt.xlabel('Position / m')
plt.ylabel('Magnitude of wave function squared')
```

7.3 Normalisation of B in solution to finite potential well

$$\psi(x) = \begin{cases} Be^{kx} & x < 0 \\ C\sin(qx) + D\cos(qx) & 0 \leq x \leq L \\ Fe^{-\mu x} & x > L \end{cases}$$

From Equations [16], [17], [18], we can rewrite this as:

$$\psi(x) = \begin{cases} Be^{kx} & x < 0 \\ B\left(\frac{k}{q}\sin(qx) + \cos(qx)\right) & 0 \leq x \leq L \\ Be^{\mu L}\left(\frac{k}{q}\sin(qL)\right)e^{-\mu x} & x > L \end{cases}$$

Our normalisation condition states that $\int_{-\infty}^{\infty} \psi(x)\psi * (x)dx = 1$, So:

$$\begin{aligned}
\frac{1}{B^2} = &\int_{-\infty}^{0} e^{2kx}dx + \int_{0}^{L}\left(\frac{k^2}{q^2}\sin^2(qx)\cos^2(qx) + \frac{2k}{q}\sin(qx)\cos(qx)\right)dx \\
&+ \int_{L}^{\infty} e^{2\mu L}\left(\frac{k^2}{q^2}\sin^2(qx) + \cos^2(qx) + \frac{2k}{q}\sin(qx)\cos(qx)\right)e^{-2\mu x}dx \\
=&\frac{1}{2k}\left[e^{2kx}\right]_{-\infty}^{0} + \left[\frac{1}{4q}\sin(2qx)\right]_{0}^{L} + \frac{k^2}{q^2}\left[\frac{x}{2} - \frac{1}{4q}\sin(2qx)\right]_{0}^{L} - \frac{k}{q^2}\left[\sin^2(qx)\right]_{0}^{L} \\
&+ e^{2\mu L}\left(\frac{k^2}{q^2}\sin^2(qx)\cos^2(qx) + \frac{2k}{q}\sin(qx)\cos(qx)\right)\left[-\frac{1}{2\mu}e^{-2\mu z}\right]_{L}^{\infty} \\
=&\frac{1}{4q^3k\mu}[2q^3\mu + q^2k\mu\sin(2qL) + 2q^3kL\mu + 4qk\mu - k^3\mu\sin(2qL) + 4qk^2\mu\sin^2(qL) \\
&+ 2q^3kcos^2(qL) + 2qk^3 + 4q^2k^2\mu\sin(2qL)]
\end{aligned}$$

We will call the right hand side of this equation X, giving us:

$$B = \frac{1}{\sqrt{X}}$$

7.4 Working for equation for probability of transmission through the finite potential barrier

$$
\begin{aligned}
T &= \left|\frac{F}{A}\right|^2 = \left(\frac{F}{A}\right)\left(\frac{F}{A}\right)^* \\
&= \left(\frac{4ikqe^{qL-ikL}}{(ik+q)^2-(ik-q)^2e^{2qL}}\right)\left(\frac{-4ikqe^{qL+ikL}}{(q-ik)^2-(ik+q)^2e^{2qL}}\right) \\
&= \frac{16k^2q^2e^{2qL}}{(ik+q)^2(ik-q)^2-(ik-q)^2(ik-q)^2e^{2qL}-(ik+q)^2(ik+q)^2e^{2qL}+(ik-q)^2(ik+q)^2e^{4qL}} \\
&= \frac{16k^2q^2}{(q^2+k^2)^2e^{-2qL}-(q-ik)^4-(q+ik)^4+(q^2+k^2)^2e^{2qL}} \\
&= \frac{16k^2q^2}{2\cosh(2qL)(q^4+2q^2k^2+k^4)-2(q^4-6q^2k^2+k^4)} \\
&= \frac{8}{\cosh(2qL)(\frac{q^2}{k^2}+2+\frac{k^2}{q^2})-(\frac{q^2}{k^2}-6+\frac{k^2}{q^2})}
\end{aligned}
$$

where we have used the hyperbolic trigonometric function:

$$\cosh(x) := \frac{e^x+e^{-x}}{2}$$

We can also use the double hyperbolic angle formula:

$$\cosh(2x) = 2sinh^2(x)+1$$

We will also use the fact that

$$
\begin{aligned}
\frac{q^2}{k^2} &= \left(\frac{2m(V_0-E)}{\hbar^2}\right)\left(\frac{\hbar^2}{2mE}\right) \\
&= \frac{V_0-E}{E}
\end{aligned}
$$

Using these expressions, we find

$$
\begin{aligned}
T &= \frac{8}{(2\sinh^2(qL)+1)(\frac{q^2}{k^2}+2+\frac{k^2}{q^2})-(\frac{q^2}{k^2}-6+\frac{k^2}{q^2})} \\
&= \frac{8}{2\sinh^2(qL)(\frac{q^2}{k^2}+2+\frac{k^2}{q^2})+8} \\
&= \frac{4}{\sinh^2(qL)(2+\frac{V_0-E}{E}+\frac{E}{V_0-E})+4} \\
&= \frac{4}{\sinh^2(qL)(\frac{2EV_0-2E^2}{E(V_0-E)}+\frac{V_0^2-2EV_0+2E^2}{E(V_0-E)}+4} \\
&= \frac{4}{\sinh^2(qL)(\frac{V_0^2}{E(V_0-E)}+4} \\
&= \frac{1}{1+\frac{V_0^2\sinh^2(qL)}{4E(V_0-E)}}
\end{aligned}
$$

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