Numerical Solutions of the Schrödinger Equation

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Abstract

The Schrödinger equation describes the wave function of a wave-particle under the influence of a force (potential). This wave function $\Psi(x,t)$ contains information about the particle including, in particular, a probability distribution of its position x at a given time t. In this project, we consider specific cases of the one-dimensional Schrödinger Equation for different forms of the potential function and solve them numerically.

Firstly, we solve the eigenvalue problem that results if the potential V is independent of time; we apply this approach to the specific case of the quantum harmonic oscillator. We next consider the anharmonic oscillator which introduces a small perturbation term to the standard harmonic model. Finally, we investigate the behaviour of the wave packet, both in free space and when acted on by a rectangular potential barrier. In all cases, we write code in MATLAB to numerically solve the problem and investigate further. Where appropriate, we also look at the analogous cases in classical Newtonian mechanics.

1. Introduction

Quantum mechanics is a relatively new theoretical framework which describes physical phenomena on the microscopic scale, in particular when Planck's constant $h \approx 6.62 * 10^{-35} Js$ cannot be assumed to be negligible. In comparison, macroscopic phenomena involve magnitudes that are large enough such that h can be set to one without appreciable error [1].

The Schrödinger equation is a fundamental equation of physics for describing quantum mechanical behavior illustrated above. In full, it is stated as

$$-\frac{\hbar^2}{2m}\nabla^2\Psi + V(x,y,z,t)\Psi = i\hbar\frac{\partial\Psi}{\partial t}. \tag{1}$$

For the scope of this project, we restrict ourselves to one dimension. Then we can rewrite the Laplacian of Ψ, $\nabla^2\Psi$ as $\frac{\partial^2}{\partial x^2}\Psi$. We explain the other parameters in detail below.

2. The One Dimensional Schrödinger Equation

2.1. Time-dependent Schrödinger Equation

For a particle of mass m constrained to move along the x-axis, the classical mechanics approach involves applying Newton's Second Law to determine $x(t)$ (the position of the particle at time t). In quantum mechanics, the Schrödinger equation determines a wave function $\Psi(x,t)$ for all time t given appropriate initial conditions [2].

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

Here, m denotes the mass of the 'particle' acted on by a potential function $V(x,t)$. $\hbar$ is the Planck's constant (h) divided by 2π

$$\hbar = \frac{h}{2\pi} \approx 1.054573 \text{ x } 10^{-34} Js.$$

According to Born's statistical interpretation of the wave function, the area under the graph of $\mid \Psi(x,t) \mid^2$ against x from a to b gives the probability of finding the particle between a and b at time t [2]. An important property of the Schrödinger equation is that if $\Psi(x,t)$ is a solution, then $A\Psi(x,t)$ is also a solution for a constant A. Furthermore, $\mid \Psi(x,t) \mid^2$ is a probability density function, thus we must find the normalizing factor A of the wave function to ensure that

$$\mid A \mid^2 \int_{-\infty}^{+\infty} \mid \Psi(x,t) \mid^2 dx = 1$$

is satisfied [2].

An indeterminacy is introduced here by the statistical interpretation, we cannot predict with certainty the outcome of a simple experiment to measure its position x.

2.2. Time-independent Schrödinger Equation

In the special case where V, the function describing the potential, is independent of time. We can use the method of separation of variables to look for solutions [3] of the form

$$\Psi(x,t) = \psi(x)f(t).$$

This gives us two ordinary differential equations:

$$\frac{\partial\Psi}{\partial t} = \psi\frac{df}{dt}, \quad \frac{\partial^2\Psi}{\partial x^2} = \frac{d^2\psi}{dx^2}f.$$

which subsequently turn the Schrödinger equation to:

$$i\hbar\psi\frac{df}{dt} = -\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi f.$$

Dividing both sides by ψf gives

$$i\hbar\frac{1}{f}\frac{df}{dt} = -\frac{\hbar^2}{2m}\frac{1}{\psi}\frac{d^2\psi}{dx^2}f + V.$$

The right hand side is a function of x alone whereas the left hand side is a function of t alone, which means both sides are in fact constants.

$$\frac{df}{dt} = -\frac{iE}{\hbar}f \tag{3}$$

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} + V\psi = E\psi \tag{4}$$

where E is defined as the separation constant,

$$E = i\hbar \frac{1}{f}\frac{df}{dt}.$$

Solving equation 3, we get:

$$f(t) = Ce^{-iEt/\hbar}.$$

Hence,

$$\Psi(x,t) = \psi(x)e^{-iEt/\hbar}.$$

Equation 4 is called the "Time-independent Schrödinger Equation" [3].

3. Eigenvalue Problem

3.1. The Hamiltonian

We now attempt to treat the equation as an eigenvalue problem. In classical mechanics, the total energy is denoted by the Hamiltonian. $\hat{H}$ is the corresponding Hamiltonian operator in quantum mechanics [4],

$$\hat{H}(\cdot) = -\frac{\hbar^2}{2m}\frac{\partial^2(\cdot)}{\partial x^2} + V(x)(\cdot).$$

In order to solve the time-independent Schrödinger equation numerically, we write it as an eigenfunction.

$$\hat{H}\psi = E\psi. \tag{5}$$

Now we can obtain E and the corresponding wave functions by finding the eigenvalues and eigenvectors of $\hat{H}$. We start by discretising the quantity $\hat{H}$ and writing it in matrix form.

Expanding the first term of $\hat{H}$ by the following process:

$$\frac{\partial}{\partial x}\psi = \lim_{\Delta x \to 0} \frac{\psi(x+\Delta x) - \psi(x)}{\Delta x} = \psi'(x)$$
$$\frac{\partial^2}{\partial x^2}\psi = \lim_{\Delta x \to 0} \frac{\psi'(x+\Delta x) - \psi'(x)}{\Delta x}$$

make the substitution $x = x - \Delta x$, then

$$\begin{aligned}\frac{\partial^2}{\partial x^2}\psi &= \lim_{\Delta x \to 0} \frac{\psi'(x) - \psi'(x-\Delta x)}{\Delta x} \\ &= \lim_{\Delta x \to 0} \frac{\lim\limits_{\Delta x \to 0} \dfrac{\psi(x+\Delta x) - \psi(x)}{\Delta x} - \lim\limits_{\Delta x \to 0} \dfrac{\psi(x) - \psi(x-\Delta x)}{\Delta x}}{\Delta x} \\ &= \lim_{\Delta x \to 0} \frac{\psi(x+\Delta x) + \psi(x-\Delta x) - 2\psi(x)}{(\Delta x)^2}.\end{aligned}$$

Replacing this by a three-point discretisation scheme:

$$\frac{\partial^2}{\partial x^2}\psi(x_n) = \lim_{\Delta x \to 0} \frac{\psi(x_{n+1}) + \psi(x_{n-1}) - 2\psi(x_n)}{(\Delta x)^2}.$$

We can now write equation 5 as

$$-\frac{\hbar^2}{2m}\frac{\psi(x_{n+1}) + \psi(x_{n-1}) - 2\psi(x_n)}{(\Delta x)^2} + V_n\psi_n = E\psi_n.$$

So we split the potential energy into N equally spaced points and write it in matrix form as follows:

$$-\frac{\hbar^2}{2m(\Delta x)^2}\begin{pmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -2 & 1 \\ & & & 1 & -2 \end{pmatrix}\begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_{N-1} \\ \psi_N \end{pmatrix} +$$

$$\begin{pmatrix} V_1 & & & & \\ & V_2 & & & \\ & & \ddots & & \\ & & & V_{N-1} & \\ & & & & V_N \end{pmatrix} \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_{N-1} \\ \psi_N \end{pmatrix} = E \begin{pmatrix} \psi_1 \\ \psi_2 \\ \vdots \\ \psi_{N-1} \\ \psi_N \end{pmatrix}.$$

We can now solve equation 4 for an arbitrary potential V. In the following section, we approach this by using MATLAB for some specific examples.

3.2. Quantum Harmonic Oscillator

In the harmonic oscillator system, the relationship between the force F and displacement x is linear. We consider the quantum harmonic oscillator by solving the Schrödinger equation

$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2 x^2\psi = E\psi, \tag{6}$$

with the potential energy $V(x) = \frac{1}{2}m\omega^2x^2$, where m is the mass of the particle and ω denotes the angular speed. [2]

The standard method to solve the differential equation in 6 - subject to auxiliary condition that $\psi(x)$ is square integrable - leads to the Hermite polynomials. In the following section, we used a numerical method to compute the energies and the wave functions. For comparison, we also used an algebraic approach in which we try to represent $\hat{H}$ as the absolute square of a ladder operator [5].

3.2.1. Dimensional Analysis of the Quantum Harmonic Equation

Computationally, we can simplify the problem by making it non-dimensional. This involves multiplying the equation by a common factor, called a length scale. We pick a suitable length scale by considering the dimensions of the existing parameters of the equation. Let

$[X]$ denote the units of the quantity X, such that we have

$$[x] = m, \qquad [m] = kg, \qquad [\omega] = s^{-1}, \qquad [\hbar] = Js = m^2 kgs^{-1}.$$

Let us define $\hat{x}$ to be the modified x such that

$$x = \hat{x}\xi, \qquad\qquad [\xi] = m.$$

The above definition implies that the quantity $\hat{x}$ is now dimensionless. We have to pick a suitable ξ such that equation 6 can be simplified and made dimensionless - one such option is $\xi = \sqrt{\frac{\hbar}{m\omega}}$ [5]. Firstly, we note that

$$\left[\sqrt{\frac{\hbar}{m\omega}}\right] = \sqrt{\frac{[\hbar]}{[m][\omega]}} = \sqrt{\frac{m^2 kgs^{-1}}{kgs^{-1}}} = \sqrt{m^2} = m.$$

Substituting for x in equation 6, we get

$$-\frac{\hbar^2}{2m\xi^2}\frac{d^2\psi}{d\hat{x}^2} + \frac{1}{2}m\omega^2\hat{x}^2\xi^2\psi = E\psi.$$

Replacing for the definition of ξ and simplifying gives us

$$-\frac{1}{2}\frac{d^2\psi}{d\hat{x}^2} + \frac{1}{2}\hat{x}^2\psi = \frac{E}{\hbar\omega}\psi = \hat{E}\psi, \tag{7}$$

where $\hat{E}$ is now the eigenvalues to be found.

We can now solve the non-dimensionalised quantum harmonic oscillator equation.

3.3. Algebraic Method

We now solve the Schrödinger equation for quantum harmonic oscillator algebraically by rewriting the equation 6 using the momentum operator $p = (\frac{\hbar}{i})\frac{d}{dx}$ [2].

We get:

$$\frac{1}{2m}[p^2 + (m\omega x)^2]\psi = E\psi.$$

To factor the Hamiltonian on the left hand side, we define a_+ the raising operator and a_- the lowering operator where

$$a_\pm \equiv \frac{1}{\sqrt{2\hbar m\omega}}(\mp ip + m\omega x).$$

Note that using the canonical commutation relation[1], we have

$$a_- a_+ = \frac{1}{\hbar\omega}H + \frac{1}{2}.$$

Thus, after rearranging, we get

$$H = \hbar\omega(a_- a_+ - \frac{1}{2}) = \hbar\omega(a_+ a_- + \frac{1}{2}).$$

We claim that if ψ satisfies the Schrödinger equation with energy E, then $a_+\psi$ satisfies the Schrödinger equation with energy $(E + \hbar\omega)$.

$$H(a_+\psi) = (E + \hbar\omega)(a_+\psi).$$

Note that the same applies to $a_-\psi$ with energy $(E - \hbar\omega)$ [2].

Applying the lowering operator repeatedly would however reach a state less than zero. At some point the machine must fail. This makes a "lowest rung" ψ_0 such that:

$$a_-\psi_0 = 0.$$

[1] $[x, p] = xp - px = i\hbar$ is known as the canonical commutation relation.

Using this and plugging in the expression for the lowering operator and p, we can determine ψ_0 from the differential equation

$$\frac{1}{\sqrt{2\hbar m\omega}}(\hbar\frac{d}{dx} + m\omega x)\psi_0 = 0.$$

Using the usual method to solve the first order ODE and then normalising it leads to

$$\psi_0(x)_{=}(\frac{m\omega}{\pi\hbar})^{\frac{1}{4}}e^{-\frac{m\omega}{2\hbar}x^2},$$

and then

$$E_0 = \frac{1}{2}\hbar\omega.$$

Simply applying the raising operator repeatedly and increasing the energy by $\hbar\omega$ with each step finally gives

$$\psi_n(x) = A_n(a_+)^n\psi_0(x) \text{ , with } E_n = (n + \frac{1}{2})\hbar\omega \text{ for } n = 0, 1, 2...$$

where A_n is the normalizing constant.
From equation 7, we note that $E_n = \hat{E}h\omega$, then

$$\hat{E}_n = n + \frac{1}{2} \text{ for } n = 0, 1, 2...$$

3.4. Numerical Solution using MATLAB

Using MATLAB, we defined a function `SCH1D_Eigen`(a, dx, b, k) that solves the time-independent Schrödinger equation for the one-dimensional harmonic oscillator. Firstly, we constructed the Hamiltonian matrix H for the eigenvalue problem by discretising potential energy between a and b into $N = \frac{b-a}{dx}$ intervals. We next found the eigenvalues $\hat{E}$ and corresponding eigenvectors ψ to solve the eigenfunction problem in Equation 5. The parameter k in our

code allows us to take the eigenvector corresponding to the kth eigenvalue. At the end of the code, we plotted the quantum probability density and the classical probability density for the kth energy state; we discuss this further in Section 3.5 below.

We produced the following table by running `SCH1D_Eigen` with $a = -10$, $b = 10$ and $k = 10$ for different values of the step size `dx` using MATLAB. We have shown the results for the first five energy values.

	n	0	1	2	3	4
stepsize = 0.1	$\hat{E}$	0.4997	1.4984	2.4959	3.4922	4.4872
stepsize = 0.05	$\hat{E}$	0.4999	1.4996	2.4990	3.4980	4.4968
stepsize = 0.01	$\hat{E}$	0.5000	1.5000	2.5000	3.4999	4.4999
stepsize = 0.005	$\hat{E}$	0.5000	1.5000	2.5000	3.5000	4.5000

From the data above, we observe that the results we get using the numerical method agree closely with the results from the algebraic method for the chosen parameters. Furthermore, we notice that the agreement gets better as the step size decreases. Ideally, to get the most accurate numerical result, we need to use sufficiently small values for the step size.

3.5. Comparing Classical and Quantum Mechanics

3.5.1. Graphical Approach

Having derived the quantum results above, we can compare the result with the analogous classical case using a graphical approach. We know that the probability of a particle being at position x at time t is given by the (suitably normalized) distribution with probability density function $|\ \Psi(x,t)\ |^2$. We can plot this for a specific energy eigenvalue using MATLAB as before.

Now for the classical case, it can be shown that the normalized probability distribution function is given by

$$P(x) = \frac{1}{\pi\sqrt{A^2 - x^2}},$$

where A is the amplitude of the harmonic oscillator [6]. We can find A by fixing a particular value for the total energy in the system - this is chosen by picking a suitable eigenvalue.

Let us pick an arbitrary E to be the total energy in the system. We know that the classical Newtonian equations give us that

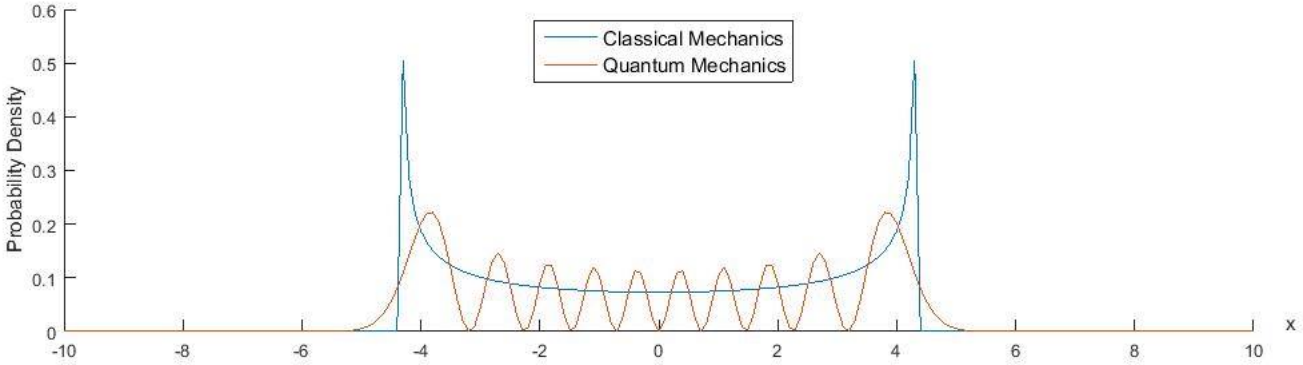
$$E = \frac{1}{2}\rho^2 + \frac{1}{2}x^2.$$

This follows from the total energy in the system being the sum of its kinetic and potential energies. At the turning points, we have maximum displacement and zero velocity (hence, zero kinetic energy), leading to

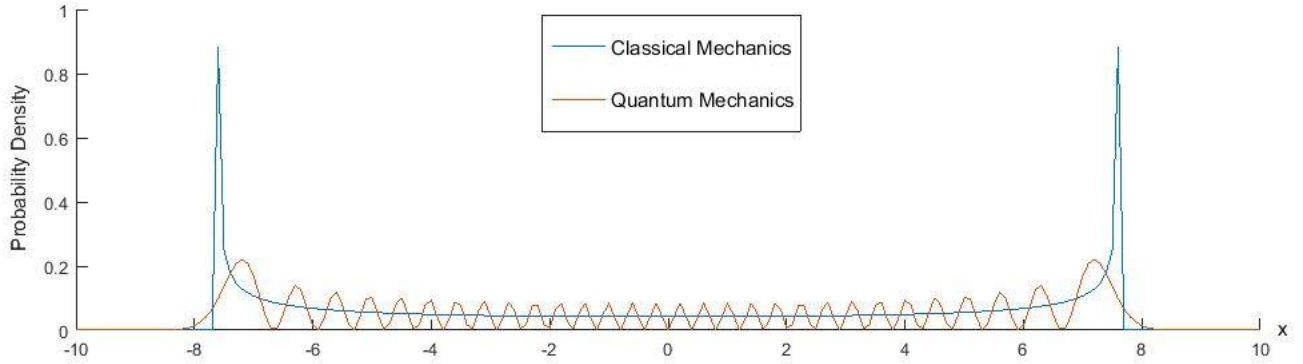
$$E = \frac{1}{2}A^2 \implies A = \sqrt{2E}.$$

Thus, we have an expression for the amplitude of the quantum oscillator in terms of the total energy in the system. We now plot the probability distribution functions for both the quantum and classical case for a fixed eigenvalue.

On the same set of axes, we plot the graphs $y = \frac{1}{\pi\sqrt{2E-x^2}}$ and $y = \frac{\texttt{psi2}}{|\texttt{psi2}|}$ where `psi2` is the square of the wave function (eigenvector) corresponding to the eigenvalue E_n. In practice, this involves picking the n^{th} row of the vector `Psi` produced by the output of our MATLAB code and squaring it. The normalisation is to ensure that the probabilities sum to 1 as per Born's interpretation [2]. The graphs are shown in Figure 1.



(a) n = 10



(b) n = 30

Figure 1: Classical (in blue) and Quantum (in red) probability distribution functions for the harmonic oscillator

The limiting case occurs as $n \to \infty$. If we smooth out the oscillations in the quantum probability distribution and overlay the classical distribution, we would get a fairly close match between the two.

3.5.2. Theoretical Explanations

There are two key points of interest when comparing quantum and classical theory:

1. *Quantised Energy Values*

   In **classical theory**, we have minimum and maximum energy values with the constituent energy taking any values in this range. The minimum value is 0, when the particle is at rest at the midpoint. The maximum value is reached at 3 points along a single oscillation - the two endpoints (maximum potential energy, zero kinetic energy) and the midpoint of the oscillation (maximum kinetic energy, zero potential energy).

   In **quantum theory**, we have a specific number of discrete, permissible energy values, given by the eigenvalues of the system as detailed above. Thus, the total energy *cannot* take any other values outside this set. This behaviour is typical of quantum states in general. We note that for our example, the energy levels are spaced linearly, i.e. $E_n \propto n$.

2. *Ground State*

   In **classical theory**, the ground state has zero energy value - this follows from the minimum energy state described above, where the particle is at rest (zero kinetic energy) at the midpoint of its oscillation (zero potential energy).

   In **quantum theory**, we note that this is not the case. The lowest eigenvalue, E_0, gives a total energy value of $\frac{1}{2}\hbar\omega$. Thus, the particle is *not* at rest in this ground state. There is a variance in the position and momentum of the particle in the ground

state, unlike in the classical case. This is consistent with the Heisenberg Uncertainty Principle - a zero energy value would allow us to fix both the position and momentum of the particle, violating the principle.

4. The Anharmonic Oscillator

4.1. Motivation

In reality, the harmonic oscillator is an idealized system to model the oscillations with a single frequency and its fundamental frequency of vibration is independent of the amplitude of the vibrations.

In comparison, the relationship between force and displacement is not linear but depends upon the amplitude of the displacement in the anharmonic oscillator system. In real life situations, materials may not be able to exert the restoring force that is directly proportional to the system's displacement. This means that the parabolic approximation is not an accurate description of the system's behaviour, hence the non-linearity. As a result, the vibration frequency can change with different displacements.

The Harmonic Oscillator can be solved analytically to get an exact solution. However, by making minor changes to the potential function, we can make our initial problem significantly more complicated. The harmonic problem simply serves to verify the accuracy of our MATLAB code by comparison with the algebraic solution. We can now adapt the same numerical method to solve the anharmonic oscillator problem. With the anharmonic oscillator, we have no analytic solution to compare with. Thus, the numerical approach we use is a best approximation to investigate this problem further.

4.2. Formulation

The anharmonic oscillator is described by the following Schrödinger equation

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+\frac{1}{2}m\omega^2x^2\psi+\alpha x^4\psi=E\psi. \tag{8}$$

We can use a similar technique as before to non-dimensionalise this equation [7]. This simplifies the equation to

$$-\frac{1}{2}\frac{d^2\psi}{dx^2}+\frac{1}{2}x^2\psi+\epsilon x^4\psi=\hat{E}\psi$$

where $\epsilon=\frac{\alpha\hbar}{m^2\omega^2}$ is a perturbation parameter and $\hat{E}=\frac{E}{\hbar\omega}$.

By transforming the above expression into matrix form, we get the corresponding Hamiltonian matrix:

$$\begin{pmatrix} \frac{1}{dx^2}+\frac{1}{2}x_1^2+\epsilon x_1^4 & -\frac{1}{2dx^2} & & & \\ -\frac{1}{2dx^2} & \frac{1}{dx^2}+\frac{1}{2}x_2^2+\epsilon x_2^4 & -\frac{1}{2dx^2} & & \\ & & \ddots & & \\ & & -\frac{1}{2dx^2} & \frac{1}{dx^2}+\frac{1}{2}x_{N-1}^2+\epsilon x_{N-1}^4 & -\frac{1}{2dx^2} \\ & & & -\frac{1}{2dx^2} & \frac{1}{dx^2}+\frac{1}{2}x_N^2+\epsilon x_N^4 \end{pmatrix}. \tag{9}$$

4.3. Perturbation Theory

For the harmonic oscillator, we were able to find the eigenvalues and eigenfunctions of the Hamiltonian in exact form. However, this cannot be done for a lot of systems in real life. We now introduce Perturbation Theory that enables us to find approximate solutions of the time-independent Schrödinger equation by building on the known exact solutions.

$$\hat{H}\psi_n=E_n\psi_n$$

Assume we know the exact solution ψ_n^0 of a simpler system with Hamiltonian $\hat{H}^0$:

$$\hat{H}^0\psi_n^0 = E_n^0\psi_n^0.$$

The difference between $\hat{H}$ and $\hat{H}^0$ (assume small) is treated as the pertubation on $\hat{H}^0$ and we are able to expand the quantities we need using Taylor Series based on the unperturbed case.

$$\hat{H} = \hat{H}^0 + \lambda\hat{H}^1 + \lambda^2\hat{H}^2 + \cdots$$
$$E_n = E_n^0 + \lambda E_n^1 + \lambda^2 E_n^2 + \cdots$$
$$\psi_n = \psi_n^0 + \lambda\psi_n^1 + \lambda^2\psi_n^2 + \cdots$$

E_n^1 is the so-called first-order correction to the energy and ψ_n^1 is the first order correction to the wave function. We will use expansions up to the first order term as it is sufficient for the anharmonic oscillator problem. By using the expansions above, we get

$$\hat{H}\psi_n - E_n\psi_n = 0 \Longrightarrow \{\hat{H}^0\psi_n^0 - E_n^0\psi_n^0\} + \lambda\{\hat{H}^0\psi_n^0 + \hat{H}^1\psi_n^0 - E_n^0\psi_n^1 - E_n^1\psi_n^0\} + \cdots = 0.$$

The terms of the same order are grouped together in brackets. These bracketed terms are linearly independent functions so the only way that the above equation can be satisfied is if the coefficient of each power of λ is zero. By setting each such term to zero, we now have

$$\hat{H}^0\psi_n^0 + \hat{H}^1\psi_n^0 = E_n^0\psi_n^1 + E_n^1\psi_n^0,$$

which we need for the derivation of the first order correction to energy. We take the inner product of above equation with ψ_n^0 [2]

$$\langle\psi_n^0|\hat{H}^0\psi_n^1\rangle + \langle\psi_n^0|\hat{H}^1\psi_n^0\rangle = E_n^0\langle\psi_n^0|\psi_n^1\rangle + E_n^1\langle\psi_n^0|\psi_n^0\rangle.$$

Since H is a complex square matrix and is equal to its own conjugate transpose, we have:

$$\langle\psi_n^0|\hat{H}^0\psi_n^1\rangle = \langle\hat{H}^0\psi_n^0|\psi_n^1\rangle = \langle E_n^0\psi_n^0|\psi_n^1\rangle = E_n^0\langle\psi_n^0|\psi_n^1\rangle.$$

Moreover, we know that

$$\langle\psi_n^0|\psi_n^0\rangle = 1.$$

In order to simplify the expressions, we use bracket notation, representing wave function corrections by their state number, so $\psi_n^0 = n$. Then, we have the fundamental result of the first order perturbation theory [8]:

$$E_n^1 = \langle\psi_n^0|\hat{H}^1|\psi_n^0\rangle = \langle n|\hat{H}^1|n\rangle.$$

This implies that the first order correction to the energy is the expectation value of the perturbation, in the unperturbed state.

In the anhamonic oscillator system, we have

$$\hat{H} = \hat{H}^0 + \lambda\hat{H}^1 = \frac{1}{2}x^2 + \epsilon x^4,$$

where $\hat{H}^0$ is the Hamiltonian matrix defined for harmonic oscillator in Equation 5.

[2] multiplying by $(\psi_n^0)^*$ and integrating

By considering the raising and lowering operator after they are non-dimensionalised, we have

$$a_- = \frac{1}{\sqrt{2}}(x + ip), \qquad a_+ = \frac{1}{\sqrt{2}}(x - ip),$$

with the properties that

$$a_-|n\rangle = \sqrt{n}|n-1\rangle, \qquad a_+|n\rangle = \sqrt{n+1}|n+1\rangle.$$

We can now apply the first-order perturbation theory to our anharmonic oscillator problem to get

$$E_n^1 = \langle\psi_n^0|\hat{H}^1|\psi_n^0\rangle = \epsilon\langle n|x^4|n\rangle$$

We can rewrite x in terms of these two operators as

$$x = \frac{1}{\sqrt{2}}(a_- + a_+).$$

When expanding the term x^4, we can see that only terms which contain an equal number of raising and lowering operators will give a non-zero contribution to the diagonal matrix element $\langle n|\hat{H}^1|n\rangle$.

We can then derive E_n^1 by

$$\hat{E}_n^1 = \frac{\epsilon}{4}\langle n|a_-^2a_+^2 + a_-a_+a_-a_+ + a_-a_+^2a_- + a_+a_-^2a_+ + a_+a_-a_+a_- + a_+^2a_-^2|n\rangle$$

Using the properties of raising and lowering operator[3] ,we can simplify the equation and get

$$\hat{E}_n^1 = \frac{\epsilon}{4}((n+1)(n+2) + n(n+1) + (n+1)^2 + n^2 + n(n+1) + n(n-1)) = \frac{\epsilon}{4}(6n^2 + 6n + 3)$$

Combining this with $E_n^0 = n + \frac{1}{2}$ we got for hamonic oscillator in section, we have

$$\hat{E}_n \approx n + \frac{1}{2} + \epsilon\frac{3}{2}(n^2 + n + \frac{1}{2}). \tag{10}$$

4.4. Numerical Solution using MATLAB

Our MATLAB code defined a function `SCH1D_Eigenh`(a, dx, b). Firstly, we constructed the corresponding Hamiltonian matrix as in 9. Next we calculated the eigenvalues of H, which represent different energy states. By using a `for` loop, we plotted a graph of different energy states against some small values of ϵ (from 0 to 0.1 with a step size of 0.01).

We plotted the results from our numerical method by running `SCH1D_Eigenh`$(-10, 0.1, 10)$; the results from the first order perturbation theory calculation 10 are shown on the same graph in order to compare the two. This is shown in Figure 2. The curves in the graph represent the numerical solution of E_n, while the dots represent the value obtained from the first order correction to E_n for different ϵ.

We observe two key features from Figure 2. Firstly, at the lower energy states, the agreement is better than at higher energy states. Secondly, we get less discrepancies for smaller ϵ. This indicates that the perturbation method is valid when the perturbation is relatively weak.

[3]
$$a_-^2 a_+^2|n\rangle = (n+1)(n+2)|n, \quad a_- a_+^2 a_-|n\rangle = n(n+1)|n, \quad a_- a_+ a_- a_+|n\rangle = (n+1)^2|n,$$
$$a_+ a_- a_+ a_-|n\rangle = n^2|n, \quad a_+ a_-^2 a_+|n\rangle = n(n+1)|n, \quad a_+^2 a_-^2|n\rangle = n(n-1)|n.$$

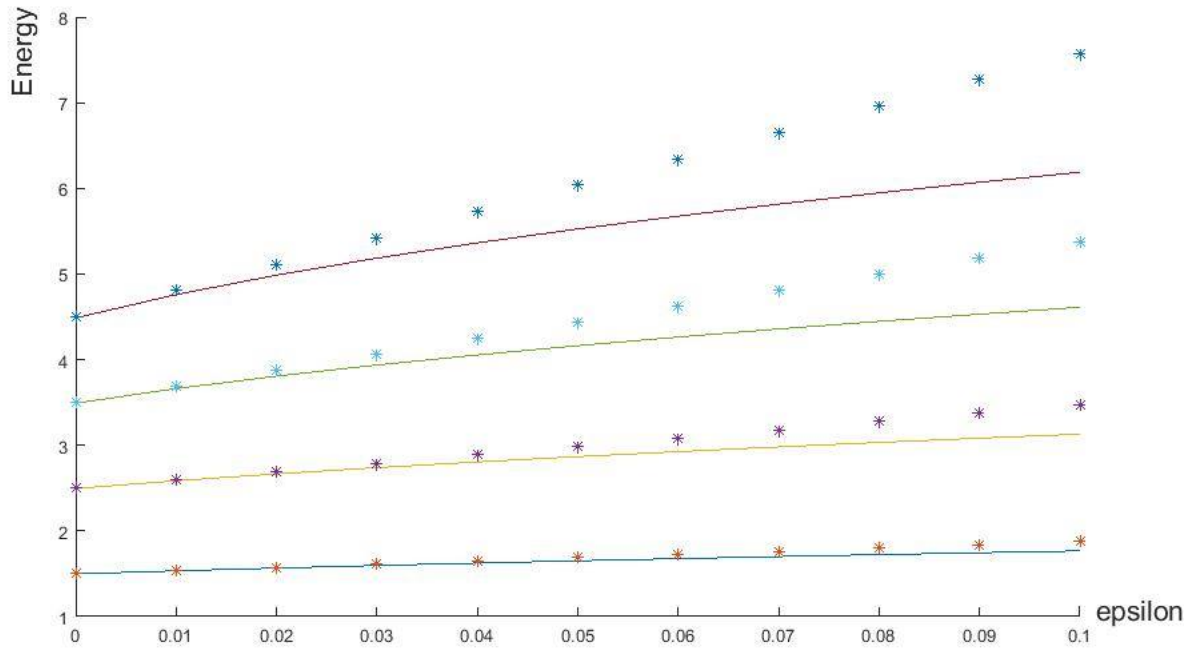


Figure 2: Energy Levels of the Anharmonic Oscillator

5. Gaussian Waves Packets and Potential Barrier

5.1. Introduction

We now turn our focus to investigate the behavior of waves. In fact, every elementary particle or quantum entity may be partly described in terms of both particles and waves. The concept of a wave packet is unique to quantum mechanics, it does not exist in the classical Newtonian model. It captures the wave-particle duality principle by providing a visual representation of the wave with a more compact "inner" wave which is sinusoidal.

The simplest case, the free particle with $V = 0$ everywhere, refers to motion at constant velocity in the classical model. In quantum mechanics, the time-independent Schrödinger equation reads

$$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi.$$

We note that again we can write $\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}$.

This gives

$$\frac{d^2\psi}{dx^2} = -k^2\psi$$

where

$$k \equiv \frac{\sqrt{2mE}}{\hbar}.$$

We write the general solution in exponential form. As there are no boundary conditions to restrict k (and hence, E), the particle can now carry any positive energy. We add on the standard time-dependence $e^{\frac{-iEt}{\hbar}}$,

$$\Psi(x,t) = Ae^{ik(x-\frac{\hbar kt}{2m})} + Be^{-ik(x+\frac{\hbar kt}{2m})}.$$

We notice that any function of x and t depend on these variables in the special combination $(x + vt)$; this represents a wave of fixed profile. Hence, $(x \pm vt = \text{constant})$ and every point on the waveform is moving along with the same velocity. Physically, this means that the shape of the wave does not change as it propagates. We now put

$$\Psi_k(x,t) = Ae^{ik(x-\frac{\hbar k^2 t}{2m})}$$

with

$$\begin{cases} k > 0 \Rightarrow \text{travelling to the right,} \\ k < 0 \Rightarrow \text{travelling to the left.} \end{cases}$$

[2].

Writing $\omega_k = \frac{\hbar k^2}{2m}$, we have that $\Psi_k(x,t) = Ae^{i(kx-\omega_k t)}$ is an eigenfunction both of $\hat{H}$ and $\hat{p} = -i\hbar\frac{\partial}{\partial x}$. We can form the general solution to the time-independent Schrödinger equation by adding together the solutions Ψ_k.

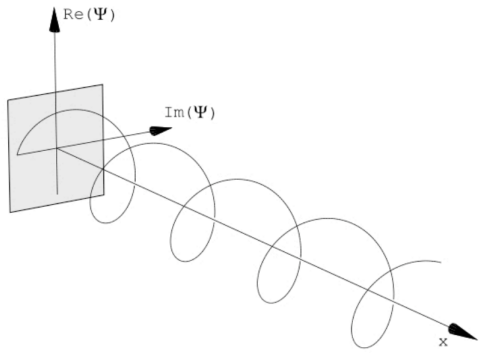


Figure 3: Diagram describing the motion of a plane wave in real and imaginary axes from the general solutions [5]

$$\Psi(x,t) = \int_{-\infty}^{\infty} C(k)\Psi_k(x,t)dk = \int_{-\infty}^{\infty} C(k)e^{i(kx-\omega_k t)}dk$$

We note that the function $C(k)$ can be any complex function of k. Thus, any $C\Psi(x,t)$ will satisfy the Schrödinger equation. The momentum-eigenfunctions Ψ_k, however, are not normalisable since

$$\int_{-\infty}^{\infty} \mid \Psi_k \mid^2 dx = \int_{-\infty}^{\infty} \mid \mathcal{N} \mid^2 dx = \infty$$

where $\mathcal{N}$ is the normalising constant.

5.2. Wave Packet

To go around this problem, we construct a wave packet which is a normalisable combination of these eigenfunctions. We choose to use the Gaussian wave packet with general wave equation:

$$\Psi(x,t) = \mathcal{N} \int_{-\infty}^{\infty} e^{-\sigma^2(k-k_0)^2} e^{i(kx-\omega_k t)}dk$$

where σ represents the standard deviation of the wave packet. For this case, we could show

that $\int_{-\infty}^{\infty} \mid \Psi \mid^2 dx$ does indeed exist.

At $t = 0$, and we write $L = k - k_0$

$$\begin{aligned}
\Psi(x,0) &= \mathcal{N} \int_{-\infty}^{\infty} e^{-\sigma^2 L^2} e^{i(L+k_0)x} dL \\
&= \mathcal{N} e^{ik_0 x} \int_{-\infty}^{\infty} e^{-\sigma^2 L^2 + iLx} dL \\
&= \mathcal{N} e^{ik_0 x} \int_{-\infty}^{\infty} e^{-\sigma^2 (L - \frac{ix}{2\sigma^2})^2} e^{-\frac{x^2}{4\sigma^2}} dL \\
&= \mathcal{N} \frac{\sqrt{\pi}}{\sigma} e^{ik_0 x} e^{\frac{-x^2}{4\sigma^2}}
\end{aligned}$$

Note that the integral is performed by shifting variables to $L' = L - \frac{ix}{2\sigma^2}$. The probability density at $t = 0$ is the Gaussian

$$\mid \Psi(x,0) \mid^2 = \mid \mathcal{N} \mid^2 \frac{\pi}{\sigma^2} e^{-\frac{x^2}{2\sigma^2}}$$

So we get the right normalisation if we take $\mathcal{N} = \frac{\sigma}{\sqrt{2\pi^3}}$, which gives:

$$\Psi(x,0) = \sqrt{\frac{1}{\sigma\sqrt{2\pi}}} e^{ik_0 x} e^{-\frac{x^2}{4\sigma^2}}$$

$$\Rightarrow \mid \Psi_(x,0) \mid^2 = \frac{1}{\sigma\sqrt{2\pi}} e^{\frac{x^2}{2\sigma^2}}$$

[9]

We can rewrite the equation with an arbitrary center x_0 by simply translating our wave packet in space. Mathematically, we can use the substitution $u = x - x_0$ to then get the following equation [10].

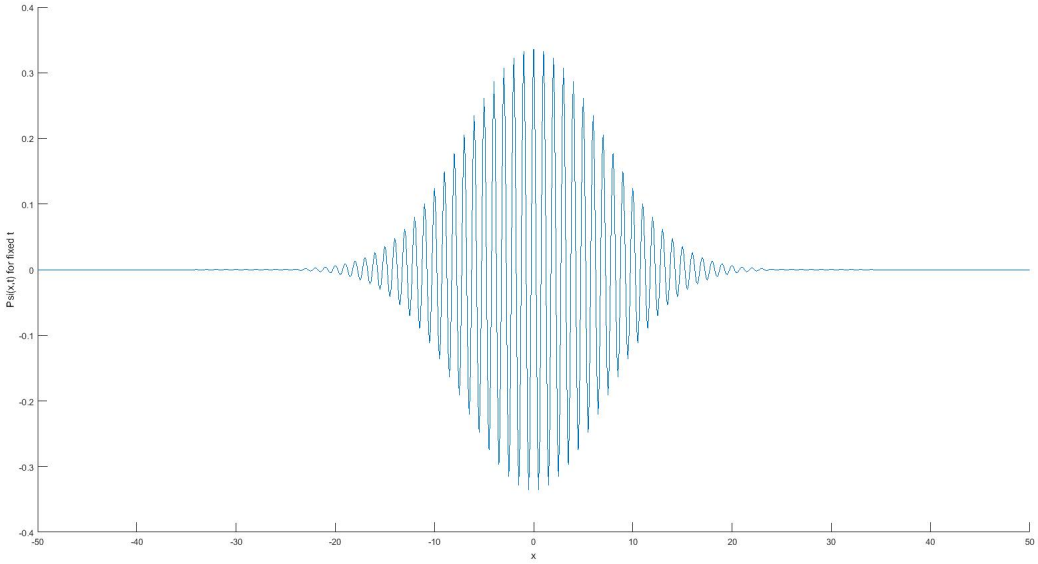
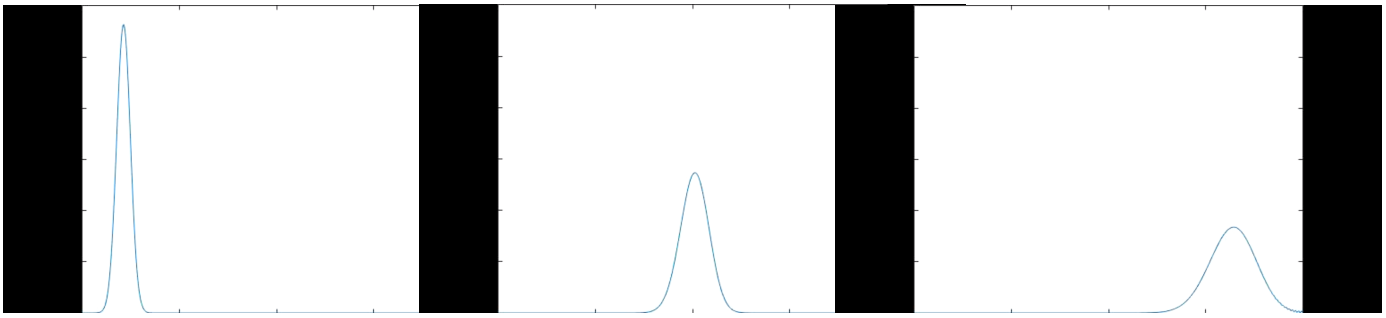


Figure 4: A Wave Packet with $x_0 = 0$, $\sigma = 5$ and $k = 2\pi \Rightarrow \lambda = 1$

$$\Psi(x,0) = \sqrt{\frac{1}{\sigma\sqrt{2\pi}}} e^{ik_0(x-x_0)} e^{-\frac{x^2}{4\sigma^2}} \tag{11}$$

A picture of the wave packet generated by our MATLAB code is shown in Figure 4. We used the code to propagate the Gaussian wave packet in time and model its dispersion. The theory shows that the profile remains Gaussian but spreads out in space. As $t \to \infty$, the peak height decreases and tends to zero. The area under the graph is conserved at all times. The code is included in Appendix C. Figure 5 shows snapshots of the wave at different times along its path.

Besides dispersing, a free-particle wave packet also translates with a speed equal to the group velocity of its de Broglie wave constituents (recall: $\lambda = h/mv$). [11]



(a) $t = 0$ (b) $t \approx \frac{T}{2}$ (c) $t \approx T$

Figure 5: The probability distribution of a wave packet dispersing for T time units

5.3. Formulation

Consider a wave packet incident upon a square potential barrier of height $V_0 > 0$ and width a from the left.

$$V(x) = \begin{cases} 0 & x < -a, \\ V_0 & -a < x < a, \\ 0 & x > a. \end{cases}$$

Starting with Equation 2, we can derive the equations that describe the time evolution of a wave packet under the influence of the potential barrier. We start by making the equation non-dimensional.

5.3.1. Dimensionless Schrödinger Equation

We use the same notation as in Section 3.2 such that $[X]$ represents the units of the quantity X. Thus, we have

$$[\hbar] = m^2 kgs^{-1}, \qquad [V] = m^2 kgs^{-2}, \qquad \left[\frac{\hbar}{mx^2}\right] = \frac{m^2 kgs^{-1}}{m^2 kg} = s^{-1}, \qquad \left[\frac{\hbar^2}{mx^2}\right] = m^2 kgs^{-2} = [V].$$

We introduce the dimensionless variables $\hat{x}$, $\hat{t}$ and $\hat{V}$ such that

$$\hat{x} = \frac{x}{L} \qquad \hat{t} = \frac{\hbar t}{mx^2} = \eta t \qquad \hat{V}(\hat{x}) = \frac{mx^2 V}{\hbar^2} = \frac{V}{V_0}$$

where L, V_0 and η are length scales. Substituting into Equation 4, we have

$$\begin{aligned} -\frac{\hbar^2}{2m}\frac{1}{L^2}\frac{d^2\Psi}{dx^2} + V_0\hat{V}(\hat{x})\Psi &= i\hbar\eta\frac{d\Psi}{dt} \\ -\frac{1}{2}\hbar\eta\frac{d^2\Psi}{dx^2} + \hbar\eta\hat{V}(\hat{x})\Psi &= i\hbar\eta\frac{d\Psi}{dt} \\ \implies -\frac{1}{2}\frac{d^2\Psi}{dx^2} + \hat{V}(\hat{x})\Psi &= i\frac{d\Psi}{dt} \\ H\Psi &= i\frac{d\Psi}{dt} \end{aligned} \tag{12}$$

where H is the non-dimensionalised Hamiltonian operator used in Section 3.2.

We can separate the variables in this equation to obtain $\Psi(x,t)$ given an initial condition

$$\Psi(x,t) = e^{-iHt}\Psi(x,0). \tag{13}$$

The initial condition is given by the original wave packet equation (11).

We now have the necessary information to solve this problem numerically in MATLAB.

5.4. Numerical Solution Using MATLAB

Using MATLAB, we defined a function `SCH1D_PB`(W, N, V, L, t) that solves the differential equation in 12 by calculating $\Psi(x,t)$, with potential energy V as defined in section 5.3. The parameter W gives the range of x, parameter N allows us to discretise the range into N intervals and L is the width of the potential barrier. We take a snapshot of the wave at time t units from the start. We produced the time propagation diagrams for an initial wave packet $\Psi(x,0)$ with a wave-number of $k = 2\pi$ and a standard deviation of $\sigma = 2$. The resulting wave packet energy is given by $E \approx \frac{1}{2}k^2 \approx 20$. We then construct the matrix H by discretising potential energy, giving us a result for $\Psi(x,t)$.

The MATLAB code also calculates transmission and reflection ratios, the 'amount' of wave either side of the barrier. We take the area under the probability distribution function in

two regions: $x < -\frac{L}{2}$ and $x > -\frac{L}{2}$. By plotting $\Psi(x,t)$ and the potential barrier, we can also see a pictorial representation of the transmission and reflection coefficients.

Figure 6 shows the case when the energy of potential barrier $V = 15$ and Figure 7 for $V = 25$. As expected, we get more transmission when the energy of the wave is higher than the potential barrier. We discuss this in further detail in Section 5.6 below.

V = 15				V = 25			
t	R	T	R+T	t	R	T	R+T
0	1	0	1	0	1	0	1
72	0.9864	0.0136	1	72	0.9891	0.0109	1
80	0.7830	0.2170	1	80	0.8855	0.1145	1
150	0.8671	0.1329	1	150	0.9993	0.0007	1

5.5. Algebraic Method

We can compare our results from MATLAB to an algebraic approach. Here, the set up is such that we have a symmetric potential barrier of height V_0 centered at the origin with total width of $2a$. First, we consider the case where the energy of the particles in the beam is greater than the height of the potential barrier (i.e. $E > V_0$. In the region with $x < -a$, we have $V = 0$, the time-independent Schrödinger Equation becomes

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi}{\partial x^2} = E\psi \tag{14}$$

$$\implies \frac{\partial^2\psi}{\partial x^2} = -\frac{2mE}{\hbar^2}\psi = -k_1^2\psi,$$

where we define $k_1 = \frac{\sqrt{2mE}}{\hbar}$.

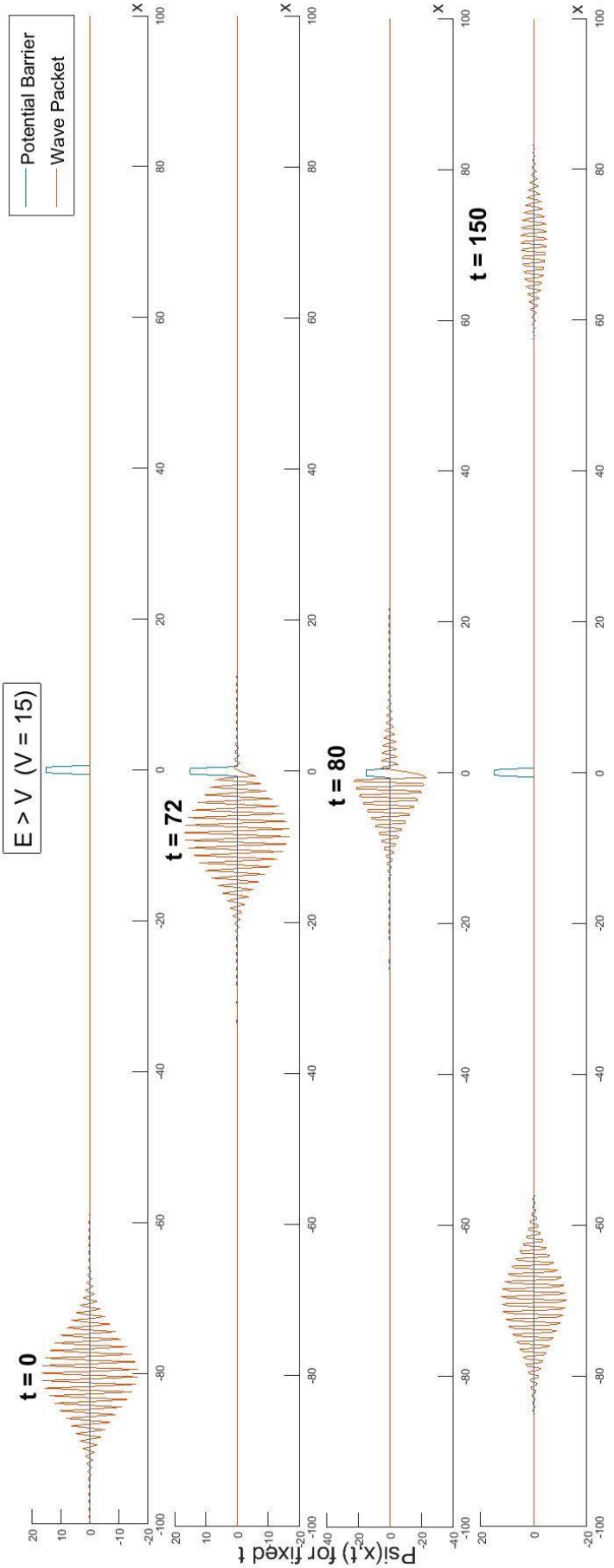


Figure 6: Time Propagation for a Wave Packet with $E > V$

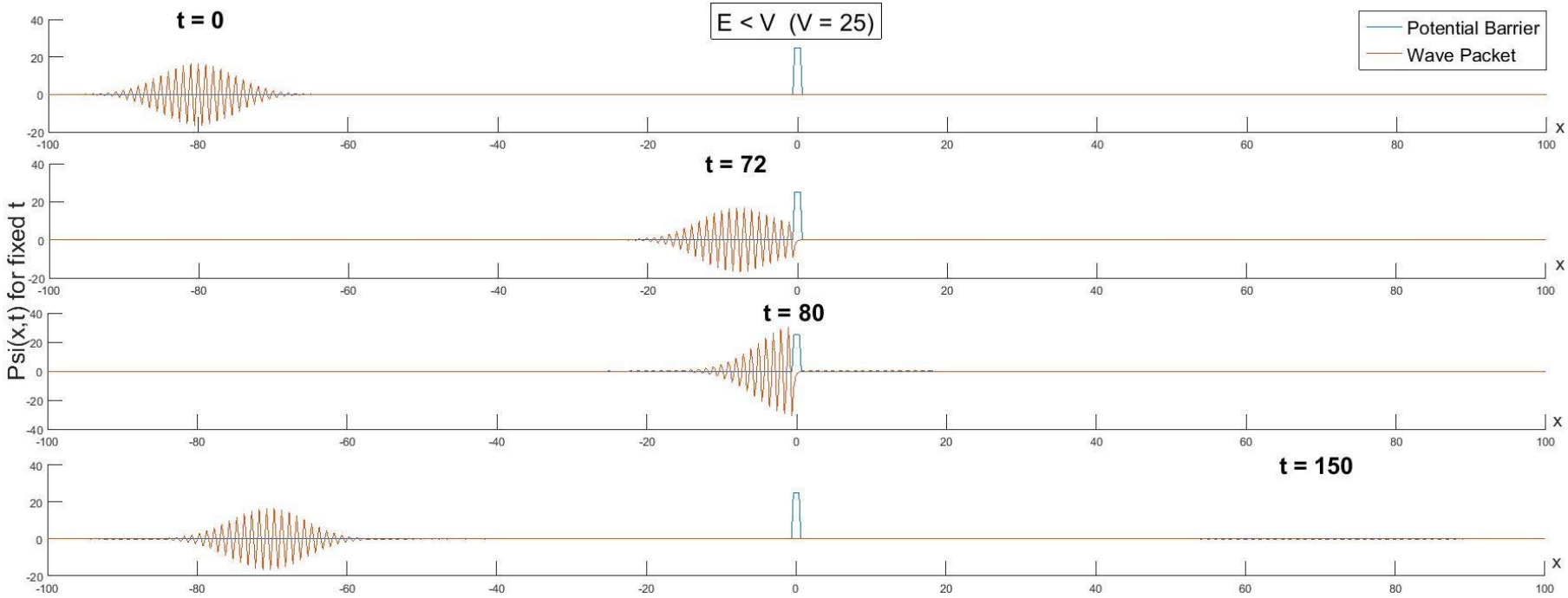


Figure 7: Time Propagation for a Wave Packet with $E < V$

In this domain the energy is entirely kinetic, we have

$$E = \frac{\hbar^2 k_1^2}{2m},$$

and the latter equation becomes

$$\frac{\partial^2 \psi}{\partial x^2} = -k_1^2 \psi.$$

Moreover in the region $-a < x < a$, with $V = V_0$ the time-independent Schrödinger equation appears as

$$-\frac{\hbar^2}{2m}\frac{\partial^2 \psi}{\partial x^2} = (E - V_0)\psi. \tag{15}$$

The kinetic energy decreases by V and is now given by

$$E - V_0 = \frac{\hbar^2 k_2^2}{2m}.$$

Where we define $k_2 = \frac{\sqrt{2m(E-V_0)}}{\hbar}$.

Therefore, for this region

$$\frac{\partial^2 \psi}{\partial x^2} = -k_2^2 \psi.$$

Similarly, for the region $x > a$, with $V = 0$, again the kinetic energy is

$$E = \frac{\hbar^2 k_1^2}{2m}.$$

Now solving for the general solutions for Equation 14 and Equation 15 we obtain

$$\psi_I = Ae^{ik_1 x} + Be^{-ik_1 x},$$

$$\psi_{II} = Ce^{ik_2 x} + De^{-ik_2 x},$$

$$\psi_{III} = Fe^{ik_1 x} + Ge^{-ik_1 x}.$$

We know that $G = 0$, because there is no wave in the opposite direction. The wave function is shown below, it can be seen pictorially in Figure 8:

$$\psi = \begin{cases} Ae^{ik_1 x} + Be^{-ik_1 x} & x < -a, \\ Ce^{ik_2 x} + De^{-ik_2 x} & -a < x < a, \\ Fe^{ik_1 x} & x > a. \end{cases}$$

Continuity at two boundaries requires that

$$Ae^{-ik_1 a} + Be^{ik_1 a} = Ce^{-ik_2 a} + De^{ik_2 a} \text{ at } x = -a,$$

$$Ce^{ik_2 a} + De^{-ik_2 a} = Fe^{ik_1 a} \text{ at } x = a.$$

The derivative of ψ is:

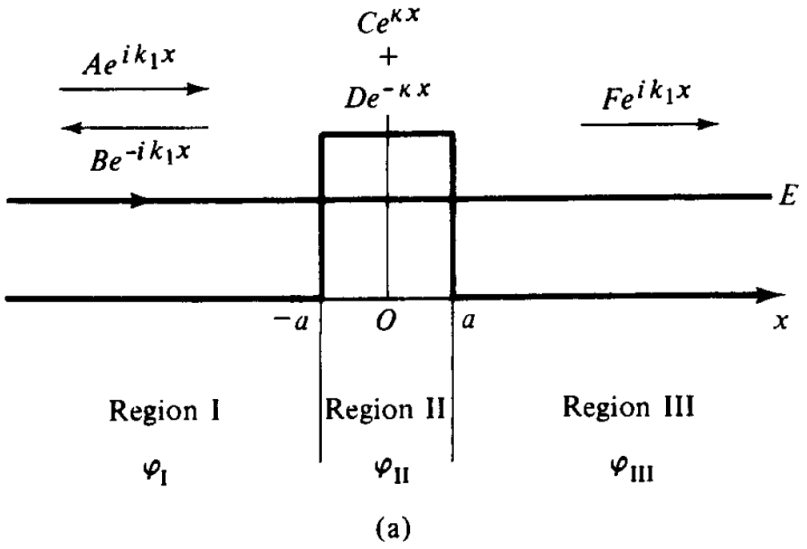
$$\psi = \begin{cases} Aik_1 e^{ik_1 x} - Bik_1 e^{-ik_1 x} & x < -a, \\ Cik_2 e^{ik_2 x} - Dik_2 e^{-ik_2 x} & -a < x < a, \\ Fik_1 e^{ik_1 x} & x > a. \end{cases}$$

Applying the boundary condition of continuity of derivative at $x = -a$ and $x = a$, we have

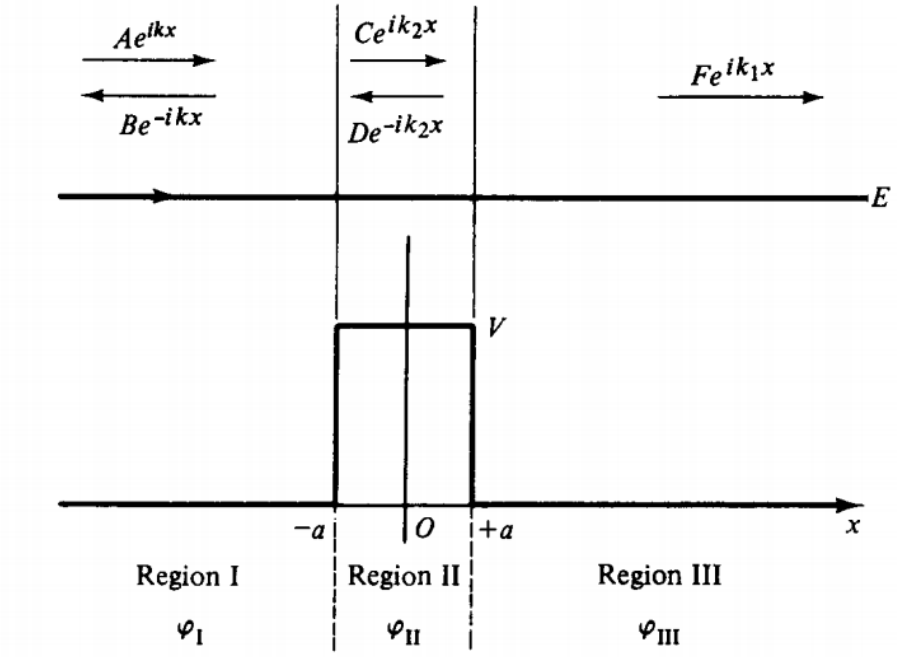
$$Aik_1 e^{-ik_1 a} - Bik_1 e^{ik_1 a} = Cik_2 e^{-ik_2 a} - Dik_2 e^{ik_2 a},$$

$$Cik_2 e^{ik_2 a} - Dik_2 e^{-ik_2 a} = Fik_1 e^{ik_1 a}.$$

We now have 4 equations and 5 unknowns (A, B, C, D, F).



(a) $E < V_0$



(b) $E > V_0$

Figure 8: Domain relevant to the rectangular-barrier scattering problem [12]

We can define the reflection and transmission coefficient as follows

$$R = \frac{\text{flux of reflected particles}}{\text{flux of incident particles}}$$

$$T = \frac{\text{flux of transmitted particles}}{\text{flux of incident particles}}$$

We get the fifth equation from this such that [12]

$$T = \left|\frac{F}{A}\right|^2, \quad R = \left|\frac{B}{A}\right|^2$$

$$T + R = 1.$$

Solving the equations above, we get the formula for T when $V = V_0 < E$ is

$$T = \frac{1}{1 + \frac{1}{4}\frac{V^2 \sin^2(2k_1 a)}{E(E-V)}}.$$

For $E < V_0$ we just simply modify the equations in the region of $V = V_0 > E$ to give

$$\frac{\hbar^2 \kappa^2}{2m} = V - E > 0.$$

In this case, the formula for T is

$$T = \frac{1}{1 + \frac{1}{4}\frac{V^2 \sinh^2(2k_2 a)}{E(v-E)}}.$$

5.6. Changes in Transmission Rate

A natural next step is to consider the Transmission ratio and investigate how it varies with L, the width of the barrier and V, the strength of the potential barrier. We approached both of these problems numerically, writing code in MATLAB to produce graphs.

Figures 10 and 9 show the graph of the Transmission ratio plotted against L, the width of the barrier. In Figure 10, this is shown for $E > V$, so we expect a higher transmission rate. The graph has a periodic nature where we get total transmission at regular intervals of L. These points occur when L happens to be a whole number of wavelengths [12].

Conversely, Figure 9 plots the same graph for $E < V$ where less transmission occurs. We see an exponential decay of transmission rate as the width of the barrier increases. As a result, much of the wave is reflected at the barrier or decays inside the barrier.

Figure 11 shows the graph of the Transmission ratio plotted against the $\frac{E}{V}$ ratio. For our code, E is fixed as we do not vary the wavenumber k. As mentioned before $k = 2\pi \Rightarrow E \approx 20$ for our wave packet. Thus for ratios less than 1, we have hardly any transmission. As $E > V$, the transmission picks up, reaching a peak between 1.5 and 2.

The numerical and analytic solutions agree fairly well for all 3 cases as can be seen. The jagged curves is a result of MATLAB's discretisation of continuous quantities. For smaller step sizes (or larger number of intervals), we can get smoother curves. However, this takes significantly longer. The graphs produced in Figures 10, 9 and 11 are a quick and easy way of verifying our code.

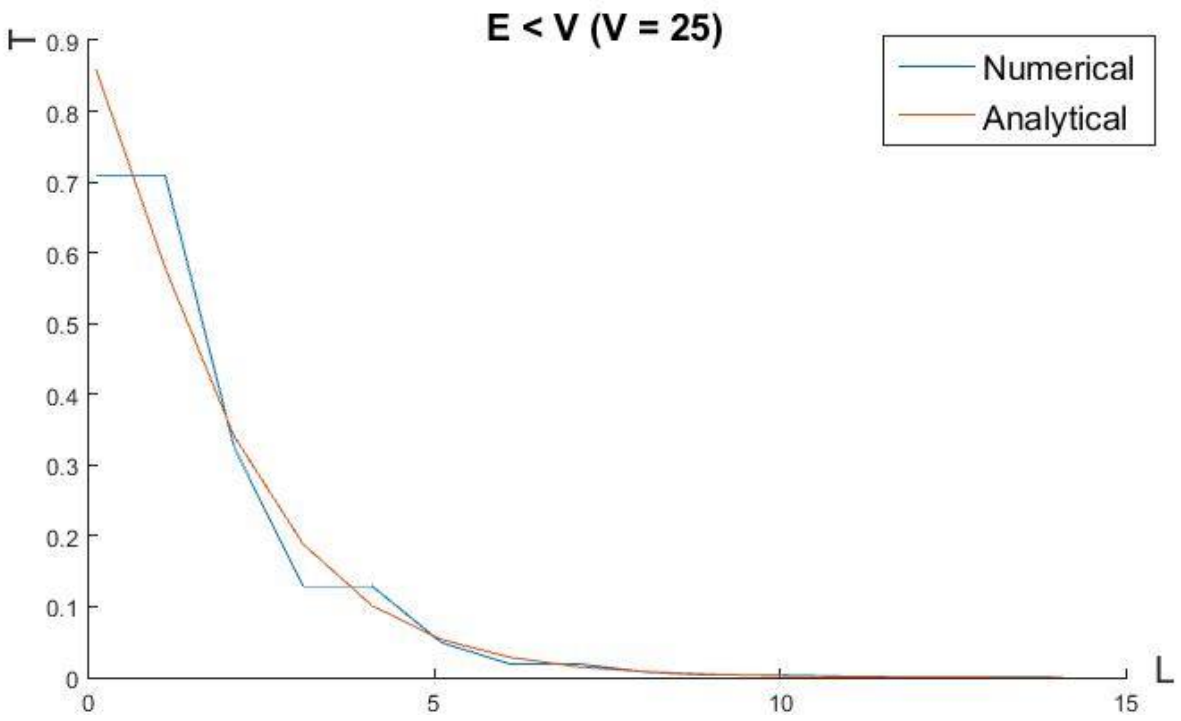


Figure 9: Transmission against L for $E < V$

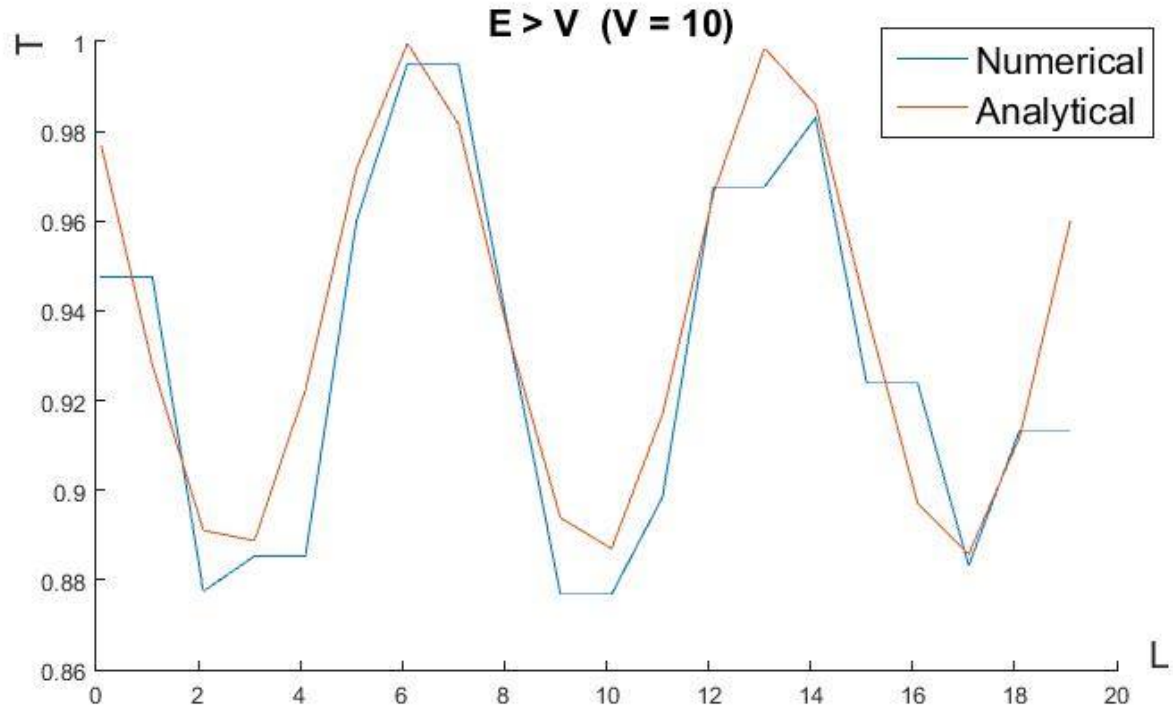


Figure 10: Transmission against L for $E > V$

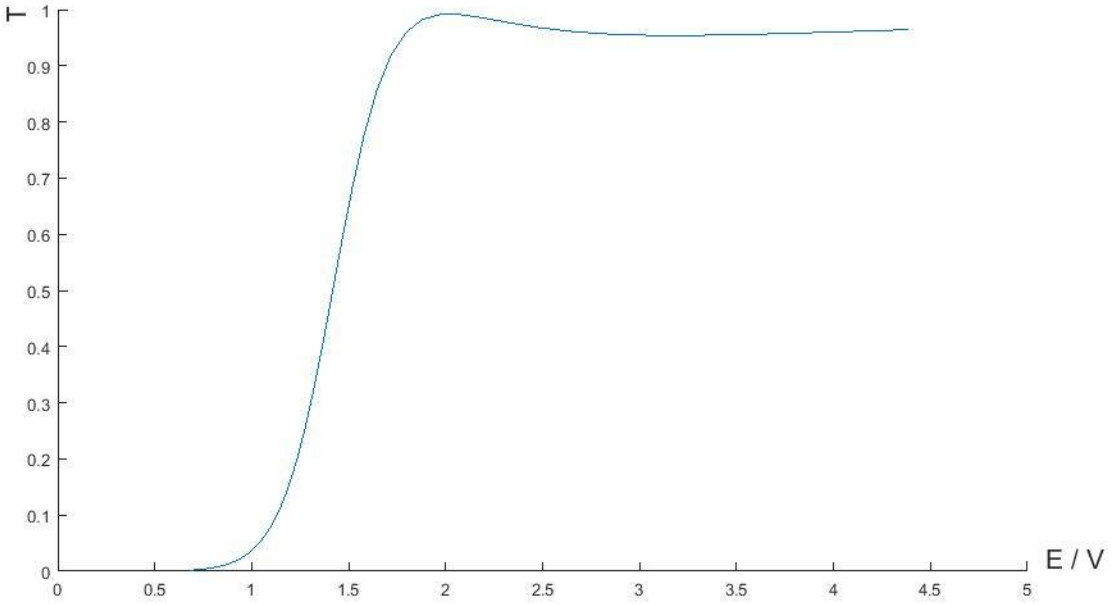


Figure 11: Transmission against the $\frac{E}{V}$ ratio

5.7. Quantum Tunneling

We now consider some of the theory regarding the quantum tunneling effect observed in scattering problems regarding the potential barrier. For classical mechanics, a particle of total energy E incident upon this barrier would always be reflected if $E < V_0$; conversely, it would always be transmitted if $E > V_0$. In quantum mechanics, both reflection and transmission happen with finite probability for positive values of V.

The phenomenon by which a wave particle with less energy than a potential barrier still crosses that barrier is called quantum tunneling. A simplistic view of this idea can be gained by considering energy changes. We can think of this as the wave particle "borrowing" energy from its surroundings; in return, the reflected wave particle has a higher energy than the incident one [13]. This energy difference ensures the conservation of energy.

The application of quantum tunneling is far reaching. It forms the basis of the scanning

tunnel microscope, where electrons tunnel through the surface to give an atomic view of a sample object. A further application lies in quantum computing, a new and exciting field of research. Unfortunately, investigating these further was beyond the scope of this project.

5.8. Variational Method

Now we switch to an alternative method to test the accuracy of our numerical solution to the Schrödinger equation, which is known as the variational method in quantum mechanics. This variational method is used to approximate the ground state energy of a system without actually solving the Schrödinger equation.

Let a system be described by a time-independent Hamiltonian H, and let ψ be any normalized well-behaved function that satisfies the boundary conditions of the problem. If E_0 is the true ground state energy of the system, then

$$\langle \psi | H\psi \rangle \geq E_0.$$

Furthermore, suppose we have a trial function ψ that is not normalized. Then multiplying by a normalization constant $\mathcal{N}$, the above equation becomes

$$|\mathcal{N}^2| \langle \psi | H | \psi \rangle \geq E_0.$$

But by definition we know that

$$1 = \langle \mathcal{N}\psi | \mathcal{N}\psi \rangle = |\mathcal{N}|^2 \langle \psi | \psi \rangle,$$

so that

$$|\mathcal{N}|^2 = \frac{1}{\langle \psi | \psi \rangle},$$

and hence our variation theorem becomes:

$$\frac{\langle\psi|H\psi\rangle}{\langle\psi|\psi\rangle} \geq E_0.$$

We now try to compare our numerical solution with the variational method by setting the potential $V = x^4$. We need to first "guess" a form for the wave function ψ. First, the function must vanish as $x \to \pm\infty$. An obvious function satisfying this would be e^{-x^2}. However, since x has units of length and we cannot take exponentials of quantities with dimensions, we would have to include a constant α with dimension of cm^{-2}. Then $e^{-\alpha x^2}$ satisfies the criteria from a dimensional standpoint. In addition, since $V = x^4$ is symmetric, we see that the eigenstates will have a definite parity. Finally, since the ground state has no nodes, it must be an even function (since an odd function has a node at the origin). Therefore, $e^{-\alpha x^2}$ has all of our desired properties [14].

The Hamiltonian is now:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + x^4$$

and hence

$$\langle\psi|H\psi\rangle = -\frac{\hbar^2}{2m}\int_{-\infty}^{\infty} e^{-\alpha x^2}\frac{d^2}{dx^2}e^{-2\alpha x^2}dx = -\frac{\hbar^2}{2m}\int_{-\infty}^{\infty} 4\alpha^2x^2e^{-2\alpha x^2} - 2\alpha e^{-2\alpha x^2}dx + \int_{-\infty}^{\infty} x^4e^{-2\alpha x^2}dx$$

As we know the integral

$$\int_{-\infty}^{\infty} e^{-2\alpha x^2}dx = \sqrt{\frac{\pi}{2\alpha}}$$

Using the integral, we can solve the other two parts. We compute and simplify $\frac{\langle\psi|H\psi\rangle}{\langle\psi|\psi\rangle}$ by using the dimensionless approach similar to above to get

$$W = \frac{\langle\psi|H\psi\rangle}{\langle\psi|\psi\rangle} = \frac{a}{2} + \frac{3}{16a^2}.$$

Putting $\frac{dW}{da} = 0$ to minimise it, we obtain the minimum value of W:

$$W = (\frac{3}{4})^{\frac{4}{3}} \approx 0.681420222$$

We now modify our numerical method to `SCH1D_Var`(a, dx, b) to obtain an approximation to the value of the ground state energy. We obtain a value of 0.667976878527490 which indeed agrees with the result we got from the variational method. Also, $\frac{\langle\psi|H\psi\rangle}{\langle\psi|\psi\rangle} \geq E_0$, once again verifying the accuracy of our approach, which gives around 2% of error. To further improve the accuracy of the approximation, we could potentially guess a different form of ψ, e.g. adding a polynomial after the Gaussian.

6. Summary

This research project successfully provides relatively accurate numerical solutions to various one-dimensional problems related to the Schrödinger equation. We consider the specific cases of the quantum harmonic and anharmonic oscillators by picking suitable potential functions.

Moreover, we visualise the propagation of wave packets, a signficant entity in quantum theory. The phenomena of the Gaussian wave packets going through a rectangular potential barrier serves as a great example to demonstrate its properties. By applying the Schrödinger equation, we were able to investigate the transmissions and reflections of the wave packets when going through the barrier.

In addition, for the problem we investigated, we could improve the accuracy of the numerical solutions by further decreasing the stepsize in the computation.

Last but not least, an approximation to the value of ground state energy is carried out to

verify our results. Further to that, there could be more ways for approximation in a quantum system, for example by using the WKB Approximation. This helps especially when some problems could not be solved directly.

There are still many aspects related to the Schrödinger Equation which we have not looked into. In particular, cases in 3 dimensions could potentially be very interesting, the jump to modify our code to solve those problems is non-trivial but certainly an extension to this project we can consider. There are further applications of quantum effects in atomic, molecular and nuclear physics, in addition to the young and exciting world of quantum computing. We hope that this research project provides a stepping stone to access these higher level problems.

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Appendix A

MATLAB code to solve the Eigenvalue Problem for the Quantum Harmonic Oscillator (Section 3.2)

```
function SCH1D_Eigen(a,dx,b,k)

% split the interval [a, b] into N equally spaced subintervals
xv = [a:dx:b];
```

```
N = length(xv);

% construct the matrix H by subdividing the given potential energy
% into equally spaced sections
main_diag = diag(1/2*xv.^2+1/dx^2);
sub_diag = -1/2*diag(ones(N-1,1),1)/dx^2;
H = main_diag + sub_diag + sub_diag';

% find the eigenvalues and the corresponding eigenvectors
[PsiX, E] = eig(H);
Energy = diag(E);

% plot on the same axes
hold on;

x = a:dx:b;
psi2 = PsiX(:,k).^2;

% classical mechanics probability distribution function
y1 = pi^(-1)*(2*Energy(k) - x.^2).^(-1/2);
plot(x,y1)

% quantum mechanics probability distribution function
y2 = psi2 / sqrt(psi2'*conj(psi2));
plot(x,y2)

xlabel('x');
ylabel('Probability Density');
legend('Classical Mechanics', 'Quantum Mechanics');

hold off;
```

```
end
```

SCH1D_Eigen.m

Appendix B

MATLAB code to solve the Anharmonic Oscillator problem numerically (Section 4.4)

```
function SCH1D_Eigenh(a,dx,b)
hold on;
% Compute energy value for different values of epsilon
epsilon = [0:0.01:0.1];
n = [1:1:5];
for k = 1:4
for i = 1:11

% Setting up free space
xv = [a:dx:b];
N = length(xv);

% Construct the Hamiltonian matrix H
main_diag = diag(1/2*xv.^2+1/dx^2+epsilon(i)*xv.^4);
sub_diag = -diag(ones(N-1,1),1)/(2*dx^2);
H = main_diag + sub_diag + sub_diag';

% Calculate the eigenvalues of H
[PsiX, E] = eig(H);
Energy = diag(E);

% Store the result into the ith column of matrix EM and ECM
EM(i,k) = Energy(n(k+1));
ECM(i,k) = n(k)+0.5+3/2 *(n(k)^2+n(k)+0.5)*epsilon(i);
```

```
end

% Plot for the same energy level against different epsilons
plot(epsilon,EM(:,k))
plot(epsilon,ECM(:,k),'*')
end
hold off;
end
```

SCH1D_Eigenh.m

Appendix C

The dispersion effect of a wave packet moving in free space. This code produces a video, screenshots are included in Figure 5.

```
function SCH1D_WPDisp(W, N, T)

% Setting up free space
x = linspace(-W/2, W/2, N)';
dx = x(2) - x(1);
dt = dx;

% Calculate the initial value of psi
% sigma = 5*sqrt(2), k = 2*pi
psi0 = sqrt(1/(5*sqrt(pi))) * exp(-((x + (W/2) - (4*5)).^2)/(2*5^2)) .* exp(1i
    *2*pi*x);

% Construct the matrix H
main_diag = -diag(1/dx^2);
sub_diag = 1/(2*dx^2)*diag(ones(N-1,1),1);
H = main_diag + sub_diag + sub_diag';
```

```
16
% Exponentiation of matrix H
18 expH = expm(1i*H*dt);
psi = expH*psi0;
20
% Plot graph of Psi^2 against x for different times t
22 writeObj = VideoWriter('dispersion.avi');
open(writeObj);
24 step = 50;

26 for t = 1:step:T
    psi = expH*psi;
28  psi2 = conj(psi).*psi;
    plot(x, 100*psi2);
30  axis([-100 100 0 12]);
    pause(0.03);
32  writeVideo(writeObj, getframe);
end
34

close(writeObj);
```

SCH1D_WPDisp.m

Appendix D

The propagation of a wave packet under the influence of a rectangular potential barrier (Section 5.3)

```
1 function SCH1D_PB(W, N, V, L, t)

3 % Setting up free space
x = linspace(-W/2, W/2, N)';
```

```
dx = x(2) - x(1);
dt = dx;

% Rectangular Potential Barrier
Vec = V*(heaviside(x + L/2) - heaviside(x - L/2));

% Calculate the initial value of psi
% sigma = 5, k = 2*pi
psi0 = sqrt(1/(5*sqrt(pi))) * exp(-((x + (W/2) - (4*5)).^2)/(2*5^2)) .* exp(1i
    *2*pi*x);

% Construct the matrix H
main_diag = -diag(1/dx^2 + Vec);
sub_diag = 1/(2*dx^2)*diag(ones(N-1,1),1);
H = main_diag + sub_diag + sub_diag';

% Exponentiation of matrix H
expH = expm(1i*H*t*dt);

% Psi and Psi^2 at time t
psi = expH*psi0;
psi2 = conj(psi).*psi;

% Transmission and Reflection Coefficients
area = psi2*dx;
R = sum(area(1:(floor((W - L)/(2*dx)))));
T = 1 - R;

% Plot graphs of V, Psi and Psi^2 against x
hold on
plot(x, Vec);
```

```
plot(x, 10*psi);
%plot(x, 100*psi2);
hold off


end
```

SCH1D_PB.m

Appendix E

The MATLAB code to work out the ground state energy value

```
function SCH1D_Var(a,dx,b)
xv = [a:dx:b];
N = length(xv);

main_diag = diag(1/dx^2+xv.^4);
sub_diag = -diag(ones(N-1,1),1)/(2*dx^2);
H = main_diag + sub_diag + sub_diag';

[PsiX, E] = eig(H);
Energy = diag(E);
Energy(1)
end
```

SCH1D_Var.m