Quantum Well Simulations in Maple

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Abstract

Quantum well Simulations have been made using Maple for educational purposes. There were three simulations showing a wave function affected by a variation of perturbations. This included an infinite well with a finite step, an infinite double well, and a well where the user may choose the amount of potential barriers. This well was shown to be accurate for varied cases, with a maximum error of $\Delta E = 6.37\%$ when taking measurements using the simulations.

The Nsteps simulation covers much of the material covered in the Quantum mechanics module given by Dr Samson at Loughborough, and can also be used to make many infinite quantum wells with potential barriers of many shapes. These simulations will be accessible to students from September 2017 via Loughborough university's student Intranet.

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1 Introduction

1.1 Motivation for Project

All second year Physics students at Loughborough university must have a grasp of the concept of quantum wells. When students are first introduced to quantum mechanics, it can be quite intimidating and in most cases, extremely challenging to understand. The aim of these simulations is to assist students with grasping fundamental concepts in the field of quantum physics. This knowledge will hopefully help the students succeed with the quantum mechanics module, and also some related modules. As an example of how this may help students in other modules, quantum wells are found in semiconductor material which is widely used in electronics, and all physics students will undertake the electronics module.

In order to assist the students with the physics course at Loughborough, the simulations created can be used to display many different types of quantum wells, few of which are important to the quantum mechanics module. Not only this, but also a problem sheet has been produced which will supplement the wells, and allow students to make the most efficient use of the simulations.

Previously, there were simulations available to the student on the Intranet, however there were needed improvements in functionality and usability. Also, there was not a double well simulation accessible to the students, and so it was important to make such an application as this well is covered in the quantum mechanics module.

These wells may also be useful for any physics student at Loughborough that wishes to improve their knowledge of wells beyond the teachings of the module, as the simulations go beyond the scope of the module.

1.2 Background

In the world observable to the naked eye, we see the laws of physics in action continuously around us. We can usually make almost perfect measurements of physical quantities like the velocity of objects, and the distance travelled using newtons equations of motion. However, when we try to make measurements on the atomic scale, things become very difficult and Newtonian mechanics are much less valuable

Max Planck developed the concept of quantum mechanics in 1900 [1], and the idea rapidly gained fame to the point where it is now widely accepted as truth. Since then, and with the help of many scientist's, quantum mechanics has now been established as the model which governs our universe.

There are many differences between quantum and classical mechanics.

On the quantum scale, Energy is not continuous; it is discrete and comes in small wave packets known as quanta. Furthermore, for a quantum state, we can only measure one observable quantity at any one time. This is due to the wave nature of particles, and is modelled by the Heisenberg uncertainty principle. For two observables; momentum p, and position x, the uncertainty principle can be written mathematically as

$$\Delta x \Delta p \geq \frac{\hbar}{2} \tag{1}$$

So in words, if we find the precise position of a particle, there will be a huge uncertainty for the momentum of the particle, and vice versa.

1.3 The Wave Function

Before we measure the location of a particle, hence causing it to collapse into one position in space, we can model all possible positions using a wave function denoted by $\Psi(x,t)$. As it is possible to find the position from this state, it is then possible to find all observable information of the system.

If we consider the singular particle's wave function which does not change with time, then the probability density P, of finding the particle in position L is denoted as

$$P = \psi(x)^* \psi(x)\big|_{x=L} [2] \tag{2}$$

and as the equation above is a probability density, it is important to make the sum of all values equal to unity. So mathematically we say,

$$\int_{-\infty}^{+\infty} \psi(x)^* \psi(x) = 1 \tag{3}$$

For a particle that is unobstructed, the wave function takes the form of a sine wave, $sinkx$ where $k = p/\hbar$. It can be seen that when we have such a wave, the momentum is known, and our position is uncertain. For any obstructed wave, we must still have a continuous wave function, but it can be made up of sinusoidal and exponential parts.

By utilising this waveform, we can find the energy of the system using the Schrödinger equation. This equation describes how the wave function of a state may evolve with time[3].

1.4 The Schrödinger Equation

The Schrödinger equation was developed in 1925 and published a year later [4]. For a quantum system, this equation is the quantum physicist's tool

when calculating the energy. To find our energy E we manipulate a wave function, $\psi(x)$. A good description of this equation can be seen in [5], where Tipler states that "the Schrödinger equation is a partial differential equation in space and time." We can write the time dependent Schrödinger equation as

$$-\frac{\hbar^2}{2m}\frac{\partial^2\Psi(x,t)}{\partial x^2} + V(x)\Psi(x,t) = i\hbar\frac{\partial\Psi(x,t)}{\partial t} \tag{4}$$

where $V(x)$ is a potential energy function. The L.H.S of the above equation can be seen as the Hamiltonian $\hat{H}$, acting on the state $\Psi(x,t)$ so for shorthand we may write

$$\hat{H}\Psi(x,t) = E\Psi(x,t) \tag{5}$$

where E is an eigen-energy value of the system.

In order to find the time independent Schrödinger equation (TISE), we follow a method from [6], known as separation of variables. The process begins by defining our state as two separate variables,

$$\Psi(x,t) = \psi(x)T(t) \tag{6}$$

So we can use Eq.(4) and Eq.(6) to find

$$\frac{1}{\psi(x)}\left(-\frac{\hbar^2}{2m}\frac{d^2\psi(x)}{dx^2} + V(x)\psi(x)\right) = \frac{i\hbar}{T(t)}\frac{dT}{dt} = E \tag{7}$$

and from there we can find the TISE to be

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + V(x)\psi(x) = E\psi(x) \tag{8}$$

For a system that is not time dependent, Eq.(8) can be used to find the energy levels of the system by use of a suitable solution, $\psi(x)$.

1.5 The 1-D Quantum Well Model

A 1-D quantum well is made up of two vertical potential barriers and a horizontal barrier, which encases the particle. The boundaries that create the outline of the well can be infinite or finite potentials. Finite barriers may also appear inside the well, for which an example of this would be a double well, or a well with a finite step.

Classically, the wave function of the particle has to be contained completely inside the well, however in the quantum world a wave function may penetrate through a finite barrier, which is a phenomena known as tunnelling. What this physically means is that there is a probability the particle can be found outside the boundaries of the well.

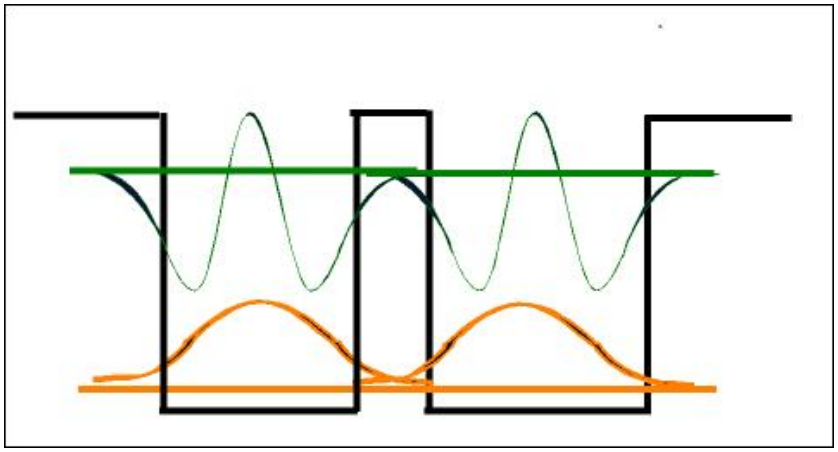

Figure 1: Quantum double well showing two different energy levels. Taken from [7].

There are many properties to a wave function inside a quantum well. Firstly, there are even and odd states inside a well. These are found by taking a line of symmetry through the middle of the well, any wave that is symmetrical is even, and anti-symmetrical means an odd wave function. In addition to this, as the particle cannot escape, infinite wells contain an infinite amount of energy levels,

Wells can be found in the real world when we have semiconductor material in between semiconductor with a wider band-gap [8]; this can then be used to create fascinating technologies such as quantum well lasers.

2 Theory

2.1 The Infinite Well

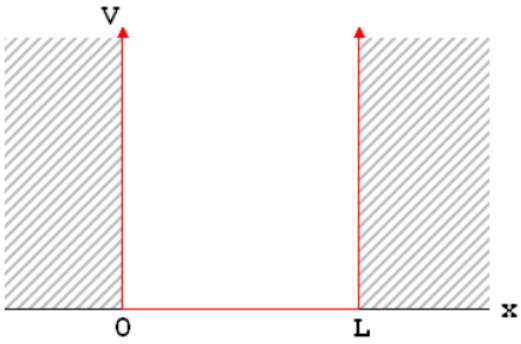

Figure 2: *taken from [9]. An infinite square well of length L.*

The infinite well is the most basic model out of all the wells. In this model we consider one particle, which occupies a discrete energy level E_n, and is governed by the wave function $\psi(x)$. The well can be seen in Fig.2, its boundaries can be described as

$$V(x) = \begin{cases} \infty, & x \leq 0 \\ 0, & 0 < x < L \\ \infty, & x \geq L \end{cases} \tag{9}$$

for a well of length L. As the well has infinite boundaries, the particle is not only classically forbidden from leaving the well, but there is also no probability of the particle tunnelling through the infinitely heightened barriers. This means that our function $\psi(x)$, must be equal to zero at these boundaries, but its spatial derivatives do not need to be continuous, as there is no wave to match onto outside of the boundaries.

Here we follow a method replicated in [10] to compute E_n by use of the TISE. We start by noticing that $V(x) = 0$, so Eq.(8) becomes

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} = E\psi(x) \implies \frac{\partial^2\psi(x)}{\partial x^2} = -k^2\psi(x)$$
$$\text{where } k^2 = \frac{2mE}{\hbar^2} \tag{10}$$

As this is a differential equation, we search for a solution in the generalised waveform

$$\psi(x) = A\cos kx + B\sin kx \tag{11}$$

where A and B are just constants. As we know $\psi(x)$ is zero at the boundaries, We can evaluate the boundary conditions. By using Eq.(11), we find that

$$\begin{aligned} \psi(0) &= A\cos k0 + B\sin k0 = 0 \\ \therefore A &= 0 \implies \psi(x) = B\sin kx \end{aligned} \tag{12}$$

and then, by evaluating the other boundary we find k to be

$$\begin{aligned} \psi(L) &= B\sin kL = 0 \\ \therefore k_n &= \frac{n\pi}{L}, \text{where } n = 1, 2, 3\ldots \end{aligned} \tag{13}$$

Now, by using Eq.(10) we can find an expression for all energy eigenstates of the infinite well

$$E_n = \frac{\hbar^2 n^2 \pi^2}{2mL^2} \tag{14}$$

and from this, we see that with a bigger box, and a heavier particle, the energy levels for the system will be lower.

In order to find the coefficient B, we apply the normalisation property shown in Eq.(3),

$$\int_0^L B^2 \sin^2 kx dx = 1 \tag{15}$$

then by integrating and some quick rearrangement, we see that

$$B = \sqrt{\frac{2}{L}} \qquad \therefore \ \psi(x) = \sqrt{\frac{2}{L}}\sin kx \tag{16}$$

Obviously there is no such thing as an infinite potential boundary, however using this model, we can acquire an idea of how an electron would behave in ideal layers of semi conductors. However, as the infinite well doesn't really have a real world application, we instead view this as a good starting point for anyone wishing to gain an understanding of quantum wells.

2.2 Infinite Well With Finite Step

Here we introduce a potential barrier to the infinite well, which can be seen in Fig.3. We know from our analysis in section 2.1 that our wave between $-a \leq x \leq b$, is given as

$$\psi_1(x) = B\sin k(x+a) \tag{17}$$

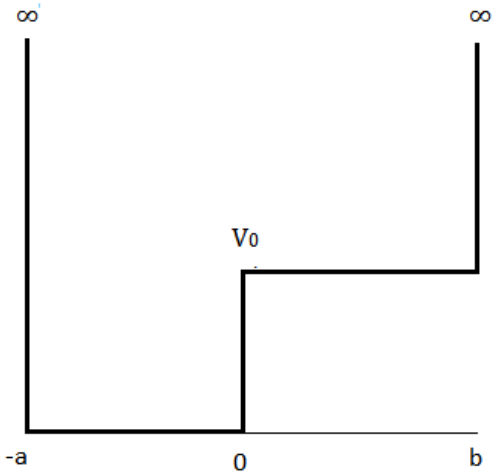

Figure 3: *An infinite square well with a potential step V_0, and of length b.*

In order to solve the TISE for the well, we must first find the wave function in the region of the well where $V(x) = V_0$. We start by using Eq.(8), and find we now have

$$\begin{aligned} -\frac{\hbar^2}{2m}\frac{\partial^2\psi(x)}{\partial x^2} + V_0\psi(x) &= E\psi(x) \\ \frac{\partial^2\psi(x)}{\partial x^2} &= -\frac{2m(E-V_0)}{\hbar^2}\psi(x) \\ \therefore K^2 &= \frac{2m(E-V_0)}{\hbar^2} \end{aligned} \tag{18}$$

Using replicated work shown in [11], we can find that there are different wave forms for the cases $E < V_0$, $E > V_0$, and $E = V_0$. Firstly, considering the case for $E < V_0$, the wave function must exponentially decay to zero at the boundary $x = b$. So we try for a solution in the general form,

$$\psi_2(x) = Ce^{Kx} + De^{-Kx} \tag{19}$$

and by applying boundary conditions, $\psi_2(b) = 0$ we see that

$$\begin{aligned} \psi_2(b) = Ce^{Kx} + De^{-Kx} &= 0 \\ \therefore C &= -D \\ \psi_2(x) = \frac{C}{2}(e^{Kx} - e^{-Kx}) &= C\sinh K(x-b) \end{aligned} \tag{20}$$

In order to find solutions for E_n, we must adopt a different approach to that of section 2.1. We solve the problem graphically, so by using the matching

conditions $\psi_1(0) = \psi_2(0)$ and $\psi_1'(0) = \psi_2'(0)$ we see that our solutions for when $E < V_0$ can be found by

$$\left.\frac{\psi_1(x)}{\psi_1'(x)}\right|_{x=0} = \left.\frac{\psi_2(x)}{\psi_2'(x)}\right|_{x=0} \implies \frac{\sin ka}{k\cos ka} = \frac{\sinh Kb}{K\cosh Kb} \tag{21}$$

$$\therefore K\tan ka = k\tanh Kb \tag{22}$$

This equation can then be used to graphically locate solutions E_n that exist below the barrier. The point of intersection can be seen in Fig.4 where we have used arbitrary values for V,a and b in Eq.(22), and with $m = \hbar = 1$.

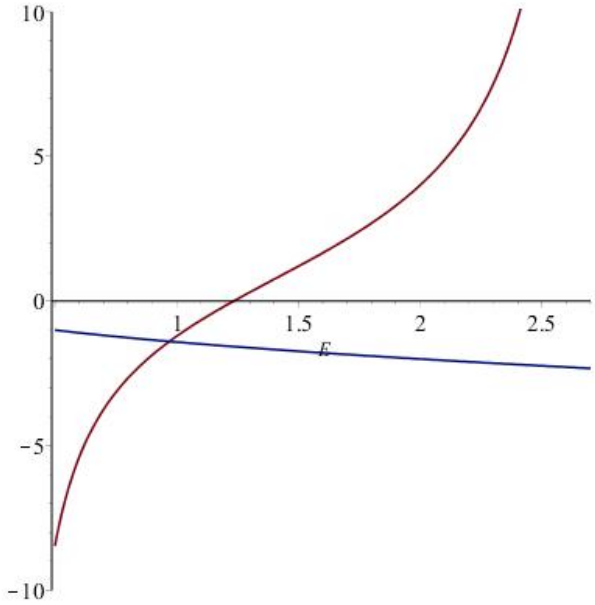

Figure 4: *The intersection point from two functions based on Eq.*(22)*. The point at which they meet is the ground state* E_0*.*

In the case of $E > V_0$, we have to make sure our wave number is not imaginary, and so it is necessary to define a new wave number,

$$q^2 = \left(\frac{2m(E - V_0)}{\hbar^2}\right) \tag{23}$$

We know that the when the energy of our wave is above the potential, there will be oscillatory motion[12] rather than exponential growth or decay. So we can now say that our wave function across the whole well for the case

$E > V_0$ is

$$\psi(x) = \begin{cases} 0, & x < -a \\ A \sin k(x+a), & -a \leq x \leq 0 \\ C \sin q(x-b), & 0 \leq x \leq b \\ 0, & x > b \end{cases} \tag{24}$$

and by repeating the steps taken for the other case, we find the matched equation to be

$$q \tan ka = k \tan(-kb) \tag{25}$$

which can be used to find energy eigenstates above the potential barrier.

For the final case when $E = V_0$, the wave function in the second region is linear, and takes the form

$$\psi_2(x) = C(x-b) \tag{26}$$

for which we can then find the final matched equation:

$$\tan ka = -kb \tag{27}$$

These were found according to the method shown in [11], for which TISE solutions are also found graphically.

Once again, as we have infinite boundaries, this well doesn't have a particular application, but the student begins to understand the concept of tunnelling and piece wise wave functions.

2.3 The Infinite Double Well

The infinite double well can be thought of as the infinite well with a finite potential step, and then another well appended to it followed by an infinite barrier. A visualisation of this can be seen in Fig.5 for which the boundaries are defined by,

$$V(x) = \begin{cases} \infty, & x \leq 0 \\ 0, & 0 < x \leq a \\ V_0, & a < x \leq b \\ 0, & b < x \leq c \\ \infty, & x \geq c \end{cases} \tag{28}$$

This variation of well has two different types of solutions, asymmetric and symmetric[13]. The wave function for the region between $0 \leq x \leq a$ is analogous to that of $\psi_1(x)$ in the previous section. In the region $0 \leq x \leq b$,

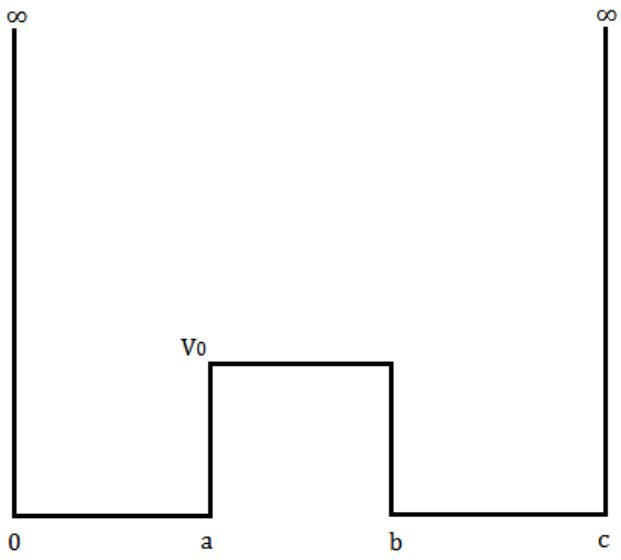

Figure 5: *An infinite double well of length c, with potential barrier* V_0.

we can see from [14], that for an asymmetric and symmetric double well, we have the respective wave functions:

$$\psi_2(x) = \begin{cases} C \sinh K(x-a) \text{ or } C \cosh K(x-a), & E < V_0 \\ C \sin q(x-a) \text{ or } C \cos q(x-a), & E > V_0 \end{cases} \tag{29}$$

In order to find the wave function in the third region, we notice that there must be oscillatory motion, and so we look for a solution in the form

$$\psi_3(x) = F \sin k(x-b) + G \sin k(x-b) \tag{30}$$

then we match this to all of the $\psi_2(x)$ wave forms. We can find all possible eigenvalues for E_n above and below V_0 via the graphical method highlighted is section 2.2. Computation of E_n will be seen later in the method section.

Although we have infinite boundaries, just by considering the middle barrier and the two separate wells, we can draw similarities to the case of electrons in semiconductor material, separated by semiconductor with a higher band-gap. Another application of the double well model is outlined in [15], where it states that a double well can be used as a quantum logic gate for ultra cold atoms confined to an optical lattice. The same paper also states

that the double well is present in the workings of an ammonia MASER. This device uses the stimulated emission of radiation via excited atoms in order to create micro waves.

2.4 N Potential Steps Well

This model is the basis of the final product of the project. A variation of the well can be seen in Fig.6. Each step may be of any height, but the first step must be set to zero. This is so we know the wave function in the first region and can therefore find the following wave functions via matching.

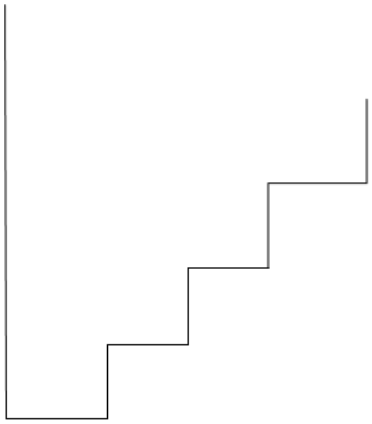

Figure 6: *A variation of the N potential steps well*

To match the waves at each step, we look to an alternative method known as the transfer matrix method. To begin, it can be seen that we have the following situation at every boundary highlighted in Fig.7. We consider a general wave function on both sides in the form $A\cos Kx + B\sin Kx$, in the region $a_{n-1} \leq x \leq a_n$, we have the wave function with known coefficients

$$\begin{aligned}\psi_{n-1}(x) = A_{n-1}\cos K_{n-1}(x - a_{n-1}) \\ + B_{n-1}\sin K_{n-1}(x - a_{n-1})\end{aligned}$$

where $K_n = \sqrt{2m(V_n - E)/\hbar}$. Also, we can say that in the region $a_n \leq x \leq a_{n+1}$, the function is defined as

$$\begin{aligned}\psi_n(x) = A_n\cos K_n(x - a_n) \\ + B_n\sin K_n(x - a_n)\end{aligned}$$

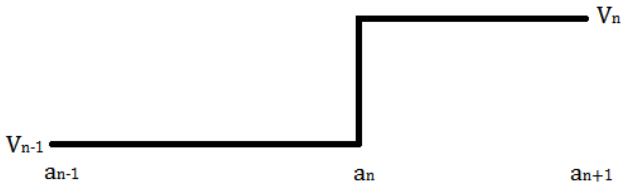

Figure 7: *The step at where* $\psi_{n-1}(a_n) = \psi_n(a_n)$

Then as we know from earlier, the matching condition is found to be

$$\left.\frac{\psi_{n-1}(x)}{\psi'_{n-1}(x)}\right|_{x=a_n} = \left.\frac{\psi_n(x)}{\psi'_n(x)}\right|_{x=a_n} \tag{31}$$

In Optics, to see how a wave travels through a medium we can use a transfer matrix denoted by T, to see how our wave will behave once it has penetrated the medium. This matrix can be defined generally as

$$T = \begin{pmatrix} \cos KL & \sin KL \\ \frac{1}{K}\frac{d}{dx}cosKx\big|_{x=L} & \frac{1}{K}\frac{d}{dx}sinKx\big|_{x=L} \end{pmatrix}$$

Using the known boundary conditions with the above equations and their derivatives stated earlier, the coefficients A_n and B_n can be found. However there is a more efficient way to solve this than using a system of simultaneous equations. Instead we can use our transfer matrix in order to find coefficients at each next step. This method can be iterated through by using a loop and arrays in order to find coefficients, and so is well suited to the problem at hand.

By using the work from Jirauschek in [16], we can use T to find the coefficients for the wave function $\psi_n(x)$, by using the relation

$$\begin{pmatrix} A_n \\ B_n \end{pmatrix} = T_{n-1} \begin{pmatrix} A_{n-1} \\ B_{n-1} \end{pmatrix} \tag{32}$$

and by creating a new constant $L = a_n - a_{n-1}$, we can define the transfer matrix T_{n-1}, as

$$T_{n-1} = \begin{pmatrix} \cos K_{n-1}L & \sin K_{n-1}L \\ -\frac{K_{n-1}}{K_n}\sin K_{n-1}L & \frac{K_{n-1}}{K_n}\cos K_{n-1}L \end{pmatrix}$$

Once these coefficients have been found, they are used with the general wave function to calculate the coefficients for A_{n+1} and B_{n+1} by using the matrix T_{n+1}. Once the coefficients have all been calculated we can then create a piecewise expression for the full wave function of the well:

$$\psi(x) = \begin{cases} A_{n-1}\cos K_{n-1}(x - a_{n-1}) + B_{n-1}\sin K_{n-1}(x - a_{n-1}), & a_{n-1} \leq x \leq a_n \\ A_n \cos K_n(x - a_n) + B_n \sin K_n(x - a_n), & a_n \leq x \leq a_{n+1} \\ \vdots & \vdots \end{cases}$$

Here we can now see that this equation can be used to describe the position wave function of a particle $\psi(x)$, confined to an infinite well with a more complex potential barrier; one example of this variation of barrier can be seen in Fig.6.

An example of this method will be seen later in the report's results section. Not only can this well be manipulated to create the wells mentioned above, but it can also be used to make multiple well structures. Structures like

this exist in superconductors[17], and are seen to realistically be modelled as multiple finite wells attached to each other.

We can also create a Kronig-Penney model [18], which is an approximation of how electrons behave in a periodic crystal lattice. This is simply constructed by creating repeatedly even sized wells.

Having said all this, the most powerful functionality of this simulation is that it has the ability to create an approximation of arbitrary potentials. So if the user wishes to analyse the behaviour of an electron about a piecewise potential, they could create it using the simulation and find all energy levels of the system. Work with an analogous idea can be seen in [19].

3 Procedure

3.1 Feasibility Study on Software

To begin production of the simulations, it was important to ensure that the optimal software to suit our needs was selected. The software needed to be able to handle piecewise functions, and allow the user to interact with simulations intuitively. With this in mind, It was decided that the two pieces of software to be investigated would be Matlab and Maple.

Maple is a mathematically based software which can be used to solve complex maths problems, it also comes with its own programming language, so that typical functionality such as IF statements and loops can be used along with logical statements. To use maple, worksheets are written and then executed.

Matlab is also designed for scientists and engineers. It is mathematically based and can be used to create a huge range of applications. It works by running a script and then interacting with a command window based on code in the script to produce any kind of output.

3.1.1 Matlab

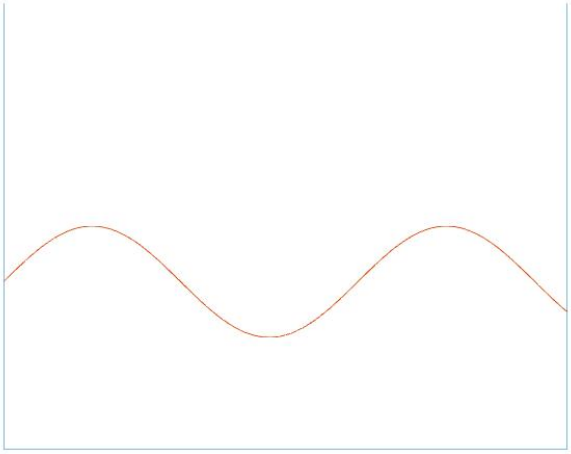

Figure 8: *An infinite well produced using Matlab, with* $n = 3$.

In order to see how Matlab would perform, an infinite well was made using the software; the code can be found in the appendix. To create the well, the script asks the user to input the well length L, and the energy level order n.

The script will then produce an exact expression for the wave function, and an image of the well which can be seen in Fig.8.

3.1.2 Maple

When investigating Maples features, the Explore command was quickly discovered and seemed to be very fitting to the task at hand. The Explore function effectively allows the user to make simulations for which variables are adjustable at run time[20]. A screen shot of what a simulation made in Maple may look like can be seen in Fig.9. Here it can be seen that by utilising the Explore command for the wave function $\psi(x) = A \sin Bx$, there has been a simulation produced, for which the parameters A and B can be adjusted until the user finds the wave form they desire.

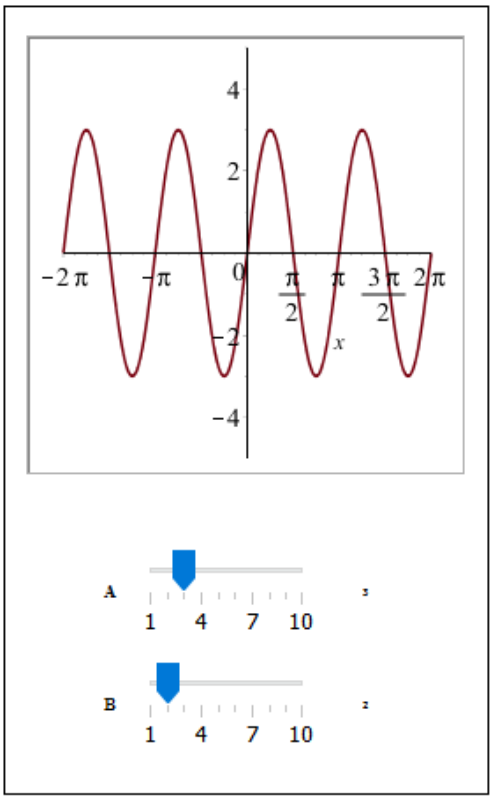

Figure 9: *An example simulation created in maple using the Explore function*

This has benefits over Matlab as these simulations allow for much more user interaction due to their ability to be adjusted at run time. Furthermore, it is extremely likely that the user will find Maple much easier to use than Matlab, due to Maple's intuitiveness. We also found that Maple would automatically change a $\sinh$ / $\cosh$ function to its respective trigonometric sinusoidal function, if it became imaginary. This proved extremely crucial for the creation of the Nsteps simulation.

For these reasons, the decision was made that Maple was clearly the more optimal candidate, and therefore the simulations were to be made using Maple.

3.2 Infinite Well With a Finite Step Simulation

This well had already been made by John Samson using maple, however the simulation was an animation and the Explore function was not used. Hence, Improving this simulation seemed like the appropriate place to start. The code for such a well had already been written by John, however the height of the potential barrier could not be changed, so there was limited interaction between student and application. The code for the well can be found in the appendix.

For the region of the well before the step, the wave function is simply $\psi(x) = \sin\sqrt{2E}x$. For the region with the barrier, A general sinusoidal wave function for $E < V$,$E > V$ and $E = V$ was matched to the previous function at $x = 1$.

As Explore was not used, the only parameter for $\psi(x)$ was E and the height of the potential barrier V was constant. So, to create a more usable application, the variable V was introduced by using Explore, allowing the size of the well to be adjusted at run time.

It can be seen that V and E are adjustable by the use of sliders. The ranges of these sliders are variable by small edition of the code, and they can also be programmed to snap to integer values only, which had been utilised for V.

The next step was to calculate and display a solution to the well (the blue line across the well in Fig.10). Using the graphical approach discussed in section 2.2, we find that have the equation

$$-\cot\sqrt{2E} = \sqrt{\frac{V-E}{E}} \qquad (33)$$

for which the values were found by using the fsolve function. This is a command in Maple that is best

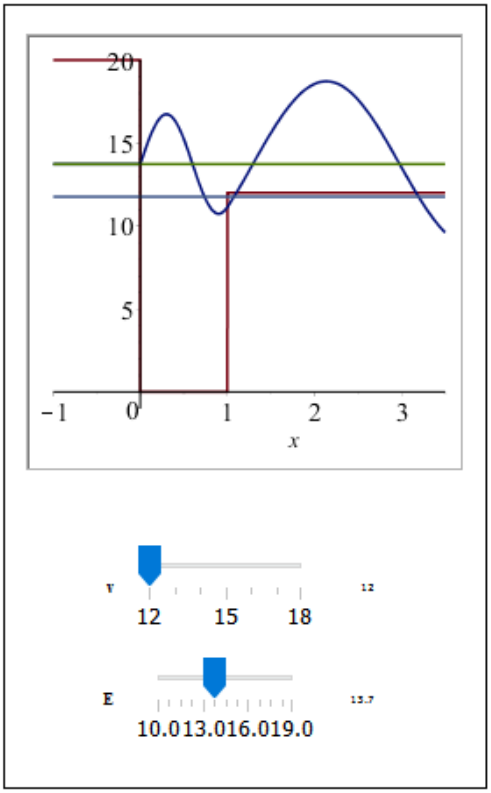

Figure 10: *Infinite Well with finite step simulation using Explore.*

defined by [21], where it states that the function solves equations by floating point arithmetic. The user can then equate the energy level to the solution line in order to view a tunnelling wave function.

3.3 Infinite Double Well Simulation

To create the double well, the first step taken was appending a well to the infinite well with a finite step. This gave us the potential boundaries necessary to accommodate the wave function, and can be seen in Fig.11; the code for the well can be found in the appendix.

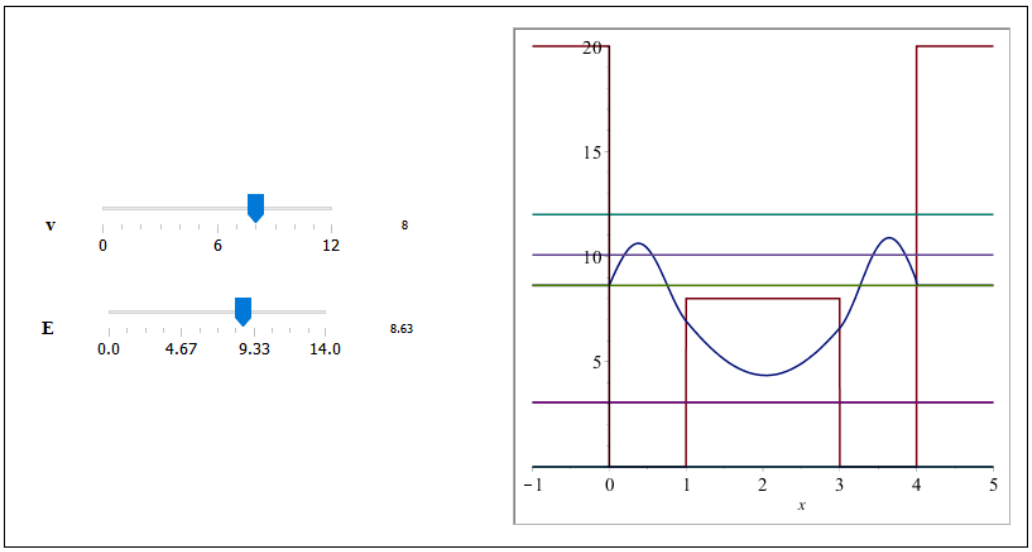

Figure 11: *Infinite Double Well simulation.*

The same steps were taken in order to create the full wave function. First, the wave from the previous simulation was taken. The three wave functions in the region $1 \leq x \leq 3$ were matched to the general wave function $A\cos kx + B\sin kx$. To mathematically calculate this, the *solve* function was used in order to produce values for A and B via simulatneous equations method. This can be seen for $E < V$ in the appendix.

The energy levels were found in a slightly different way as for a double well there are symmetrical and asymmetrical solutions. In order to find the symmetrical solutions, we use the boundary condition

$$\sin k = \cosh K \qquad (x = 1) \tag{34}$$

and then followed the method shown in section 2.2. Then to find the asymmetrical solutions, we use the condition

$$\sin k = \sinh K \tag{35}$$

These are then plotted using the fsolve command for which code can be found in the appendix.

3.4 The Nsteps Simulation

To create this well a different approach from previous was adopted. This time, the user may input the mass m, and input the height of the all the steps into the V_n array or input pre-set heights by use of the buttons shown in Fig.12.

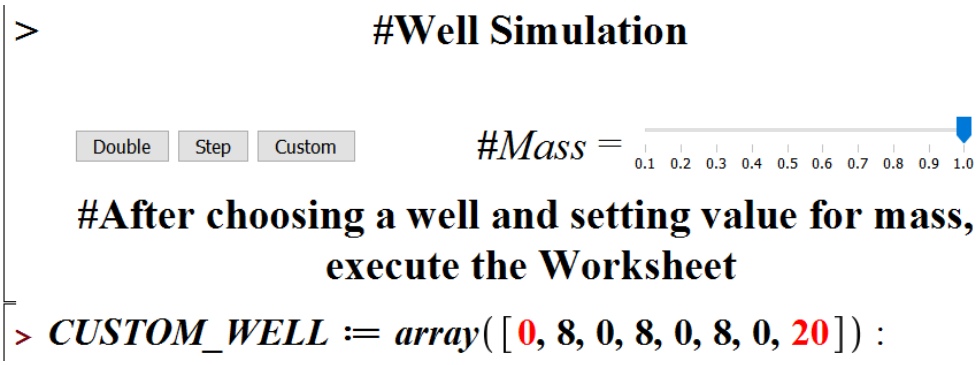

Figure 12: *Input controls for the Nsteps simulation.*

The amount of steps is limited to 8, due to processing time when calculating coefficients. After the user has chosen values for the input parameters, these values are processed in a loop, which creates the potential well, and the wave function.

To create the wave, we use a transfer matrix, T. Where $L = a_n - a_{n-1}$ and $K_n = \sqrt{2(m(E - V_n))}$, we utilise the transfer matrix

$$T = \begin{pmatrix} \cos K_{n-1}L & \sin K_{n-1}L \\ -\frac{K_{n-1}}{K_n} \sin K_{n-1}L & \frac{K_{n-1}}{K_n} \cos K_{n-1}L \end{pmatrix}$$

to find the coefficients for the wave function at the next step by using the equation below:

$$\begin{pmatrix} A_n \\ B_n \end{pmatrix} = T \begin{pmatrix} A_{n-1} \\ B_{n-1} \end{pmatrix} \tag{36}$$

These are then applied to a general wave function, and then the loop begins the next iteration. The output of this can be seen in Fig.13 and the code for the loop can be found in the appendix. Course and fine controls have been introduced in order to ease the process of finding a solution.

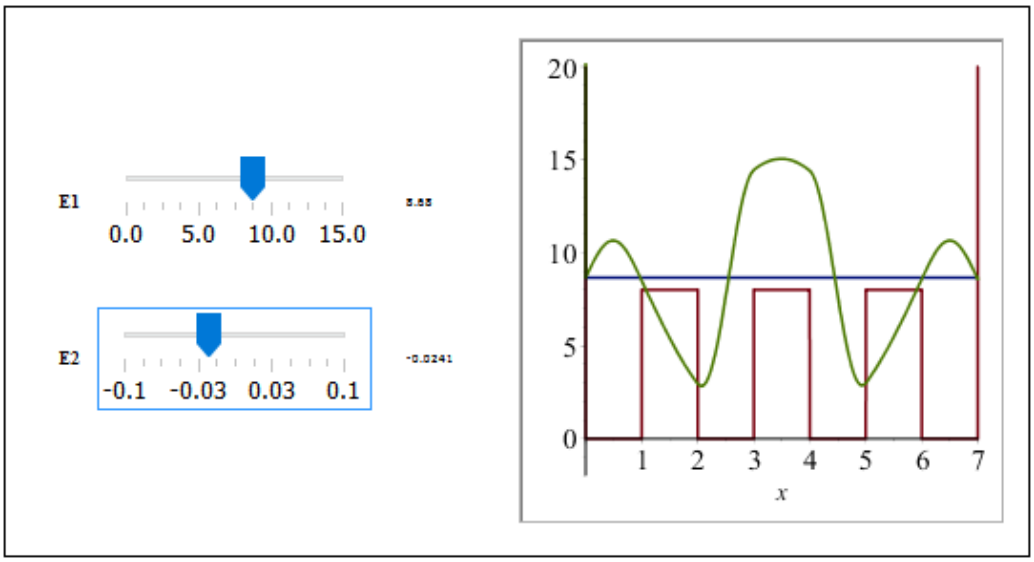

Figure 13: *The Nsteps simulation with a custom input for all V_n.*

3.5 Problem Sheet for Wells

To promote use of the Nsteps well, it was important to make a problem sheet to help guide the students and allow them to make the most efficient use of the simulations. Not only this, but the problem sheet had to also relate what the simulations display to the underlying physics of quantum wells.

The sheet came with brief instructions on how to use the simulation, and asks the user to draw specific energy levels. The sheet then asks how the outputs compares to classical physics, which is all in suit with the specification of the module. There is also a final question which goes beyond the scope of the module and challenges the student, making them think for themselves as there are no notes on the wells the students are queried on in the final question. The sheet can be found in the appendix.

4 Results and Discussion

4.1 Operating the Simulations

4.1.1 Infinite Well With Finite Step and Double Well Simulation

Both of these simulations are operated in a similar way. To begin, the user must execute the whole worksheet, then the application becomes active. After this, the user may scale through different heights of potential barrier, and then adjust the energy of the wave function until a solution is found. The simulations are limited at a height of $V = 20$, as this is the height the infinite boundaries are set at.

The infinite well with a finite step shows an energy level for the first excited state E_1, because this energy level best shows the tunnelling through the barrier, as there is exponential decay towards $\psi(x) = 0$. In addition, when trying to find the energy level E_0, much fine tuning is required as the wave function changes rapidly about this point. This is why the fine and coarse controls were implemented for the Nsteps simulation.

The infinite double well shows four solutions in total, two symmetrical, and two anti-symmetrical. If we set the barrier to $V = 0$, it simply becomes an infinite well, and by changing the height of the barrier, we can see how a perturbation effects a simple quantum system. To find a solution to this well, the wave function must equal zero at the right hand boundary.

A more experienced maple user can edit the range of the sliders in order to fine tune a solution. They may also want to see how a non-integer heightened barrier is tunnelled through, but they may not set the perturbation to a higher height than the boundaries of the well.

4.1.2 Nsteps Simulation

The function of this well has some differences to the other two wells. To first step of using the simulation is setting the mass using the slider, which is a functionality added in order to give the problem sheet an extra few questions to ask the student. It was decided that the mass would be ranged between $0.1 - 1.0$, this was to keep the wave functions from being too erratic, but still allow the student to see effects of changing the mass of a particle in a well.

The user can then select one of three buttons, "Step" which is the infinite well with a finite step, "Double" is the infinite double well, and "Custom". the Custom button allows the user to set different heights of each step in an array shown below the buttons; this can be seen in Fig.13. To shorten the well, the user can set the appropriate element V_n to 20, and the well will be infinite from there onwards. There is also the option to change the length of

each step, however this is not needed for the problem sheet, and so it is left for more adept Maple users to utilise.

After this, the final step is to execute all the worksheet, causing the application to become active so that energy levels of the created well can be found.

Despite this, there are limitations to this simulation. Firstly, we cannot change the height of each step after execution. This is because variables cannot be passed through using an array, however it is still easy to change the height of the steps. Furthermore, as stated earlier the amount of steps is limited to eight as processing time increases exponentially with each step. For the average computer when we have more than eight steps, this period of time is too long. The well can only handle horizontal steps, but these steps can be shortened to create approximate diagonals through staircase sequenced steps. The biggest limitation though is that the end boundaries of the wells must be infinite, and the first step must be equal to zero. This doesn't allow us to have a finite boundary on the left side, so we cannot create a finite well.

4.2 Use of the Infinite Double Well Simulation

To give an example of how the double well simulation can be used, two energy levels, E_1 and E_2 were compared to see how this simple perturbed system behaves.

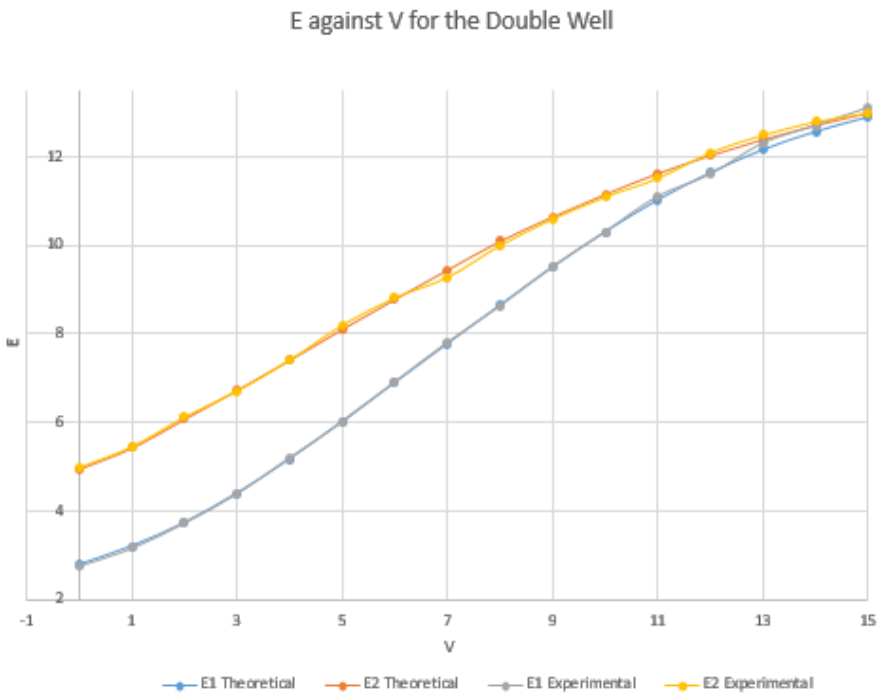

Figure 14: *Graphs showing how a potential barrier in an infinite double well affects the energy levels.*

These energy levels were chosen as neighbouring levels within a double well, which are with and without symmetry, come closer together as the potential barrier height is increased. Here, E_1 is the symmetric energy level and E_2 is anti-symmetrical.

The results show that the double well simulation can accurately find the energy levels for a large range of potential barrier heights. However, when we try to evaluate the levels beyond potentials of height $V = 13$, the simulation struggles to predict correct values. This is mainly down to the lack of intricateness of the controls. To fix this, a fine control could be added to the simulation, so that the controls work in an analogous fashion to the Nsteps well.

4.3 Accuracy of The N Steps Simulation

After use of the simulations controls, it was estimated that the human error and hence the total error for finding solutions was $\Delta E = \pm 5\%$.

4.3.1 Infinite well With finite step

When measuring the accuracy, only the Nsteps well was used as this can be used to form all wells previously mentioned. It is also only necessary to use this well as this is the final product of the project, and will hence be the well available to the students next year and onwards.

Below is a table for the infinite well with finite step energy levels E^e, where the e superscript denotes these results were found experimentally(by use of the simulation). We compare these to the theoretical values E^t, with constants $m = 0.1$ and $\hbar = 1$ for simplicity. To find value of E^t, Eq.(22) and Eq.(25) were used in combination with the fsolve Maple command; the proof can be found in the appendix.

V	E_0^e	E_1^e	E_0^t	E_1^t
5	2.89	7.42	2.89	7.48
6	3.06	8.29	3.05	8.29
7	3.21	9.11	3.20	9.10
8	3.30	9.84	3.31	9.89
9	3.41	10.6	3.41	10.6
10	3.50	11.3	3.50	11.4
11	3.58	11.9	3.57	12.0
12	3.63	12.6	3.64	12.6

Table 1: *A table to show experimental and theoretical Energy levels for different sized potential steps in an infinite well with a finite step.*

It is quite clear from Table 1 that the well predicts the energy levels almost perfectly, so no plot is needed. Also, the only error present is due to personal judgement of when $\psi(x) = 0$ at the far boundary of the well. The user may increase the precision of the simulation by making the range of $E2$ smaller, however the measurements taken above were rounded to three significant figures. Maximum error of measuring E, using the simulations, was for E_1 when $V = 5$, and was found to be 0.8%. This difference was likely due to the human error in judgement of when the simulation was displaying a solution.

4.3.2 Infinite Double Well

Here the first value of our independent variable was $V = 6$ instead. This was so that we could evaluate both a symmetric E_{sym}, and asymmetric energy level E_{asym} for when $E < V$. Again we have the constants $m = 0.1$ and $\hbar = 1$. The results of the testing of this well can be seen in Fig.15. Error bars were

not displayed on these graphs as it was too insignificant when compared to the range of the data. Also no units are shown as we have arbitrary units. The experimental symmetrical energy levels were almost exactly the same as

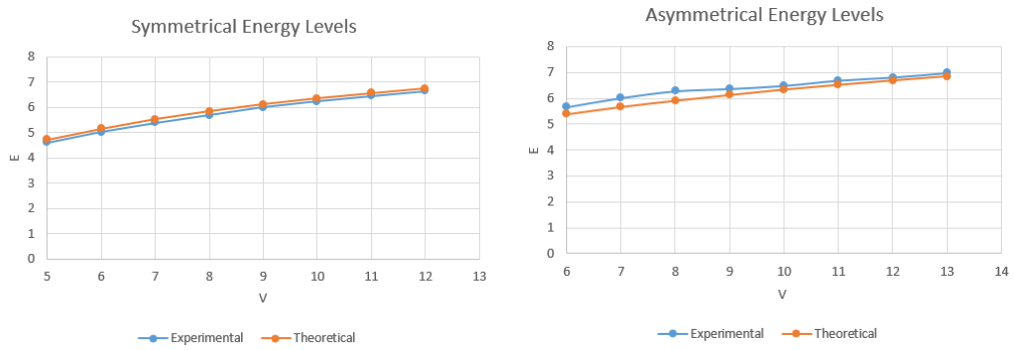

Figure 15: *Graphs comparing the experimental and theoretical energy level values for an infinite double well made using the N steps simulation.*

what was theoretically predicted, with approximately only a 0.1 difference between the values predicted and those found. Considering this, it can be said that the well finds symmetrical values to a high standard for a substantial range of V.

For the asymmetrical energy levels, experimental values in the range $V > 10$ matched up well, but further testing would be needed in order to see if this relationship stayed true. The main discrepancy is for the height $V = 8$, where there is a 0.4 difference between predicted and experimental. Some of this value could find contributions from error in finding $\psi(x) = 0$ at the boundary on the right. However the rest could be down to the theoretical solutions being found graphically instead of exact. Even this is the maximum amount of error in E for any V, it still only equates to 6.37% error, so the simulation cannot be seen as faulty.

Overall it can be said that the Nsteps well can be used to create a double well and find energy levels to a high degree of accuracy.

5 Conclusion

In summary, the project was a huge success exceeding expectations, with key learning resources being created for the students. All the simulations have been proven to function with a high degree of accuracy, with a maximum error margin of 6.37%. Not only are the energy levels calculated accurately, but the wave functions created look identical in shape to those found by scientists.

Despite limitations to the usability of the Nsteps potential well, the simulation is still a great success and can be used to create a huge variety of wells. The simulation can display all wells covered in the physics modules at Loughborough university. Not only has the simulation fulfilled all initial requirements of the project, but it can also be used to create approximations of any kind of arbitrary infinite well. Therefore this is not only a powerful tool for students wishing to further their knowledge of quantum mechanics, but to scientists who find themselves wishing to visualise a wave function through a complex variety of well.

Furthermore, the problem sheet which accompanies the simulations helps the students make full use of the wells. It allows the students to create important wave functions, and compare them to different energy levels or the same level with different values for mass and perturbation height. Moreover, the problem sheet reaches beyond the scope of the module, helping them to use initiative and become better physicists.

6 Acknowledgements

I would like to thank John Samson for all his guidance throughout the duration of the project. He was a great help and made an extra effort to assist with the project whenever available.

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7 Appendix

```
x= 0:0.001:L;
y1=zeros(size(x));
A=sqrt(2/L);
for i = 1:1:length(x)
    if x(i) <=L
      y2=(5*A)*sin(n*(3.14159*x)/L)+10;
        y1(i) =2    ;
    end
end
plot(x,y1,x,y2);
ylim([2 20]);
line([0 0], ylim);
line([L L], ylim);

grid off;

s= sprintf('particle in a box where n=%d',n);
sprintf('the wave function is phi = %d *sin(%e*pi*x)/%f',A,n,L)
title(s)
axis off;
```

Figure 16: *Matlab code for the infinite well.*

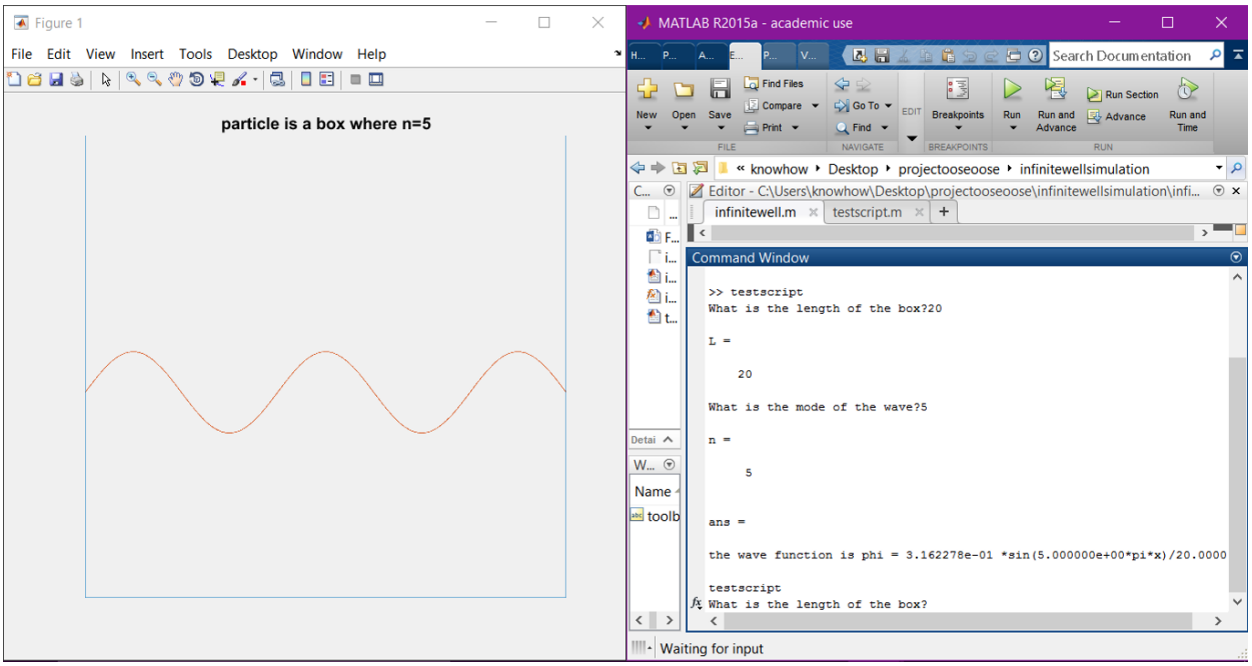

Figure 17: *Example of user interaction with program and output produced by Matlab.*

```
> p(E) := -cot(sqrt(2E))
```

$$p := E \to -\cot\left(\sqrt{2E}\right)$$

```
> l(E, v) := sqrt((v - E)/E)
```

$$l := (E, v) \to \sqrt{\frac{v - E}{E}}$$

```
> Q(v) := fsolve(l(E, v) = p(E), E = 10 ..15)
```

$$Q := v \to fsolve(l(E, v) = p(E), E = 10 \,..15)$$

```
> 
>
>
> Explore(plot([piecewise(x < 0, 20, 0 < x < 1, 0, 1 < x, v), piecewise(x < 0, 0, 0 < x < 1, sin(sqrt(2E)x), x > 1, piecewise(E < v,
      sin(sqrt(2E))·cosh(sqrt(2(v - E))·(x - 1)) + sqrt(E/(v - E))·cos(sqrt(2E))·sinh(sqrt(2(v - E))·(x - 1)), E = v, sin(sqrt(2E))
      + sqrt(2E)·cos(sqrt(2E))·(x - 1), E > v, sin(sqrt(2E))·cos(sqrt(2(E - v))·(x - 1)) + sqrt(E/(E - v))·cos(sqrt(2E))·sin(sqrt(2(E
      - v))·(x - 1)))·3 + E, E, Q(v)], x = -1 ..3.5, view = -1 ..20), parameters = [v = 12 ..18, E = 10.00 ..19.00])
```

Figure 18: *Code for infinite well with finite step. Also shows the code for the solution line.*

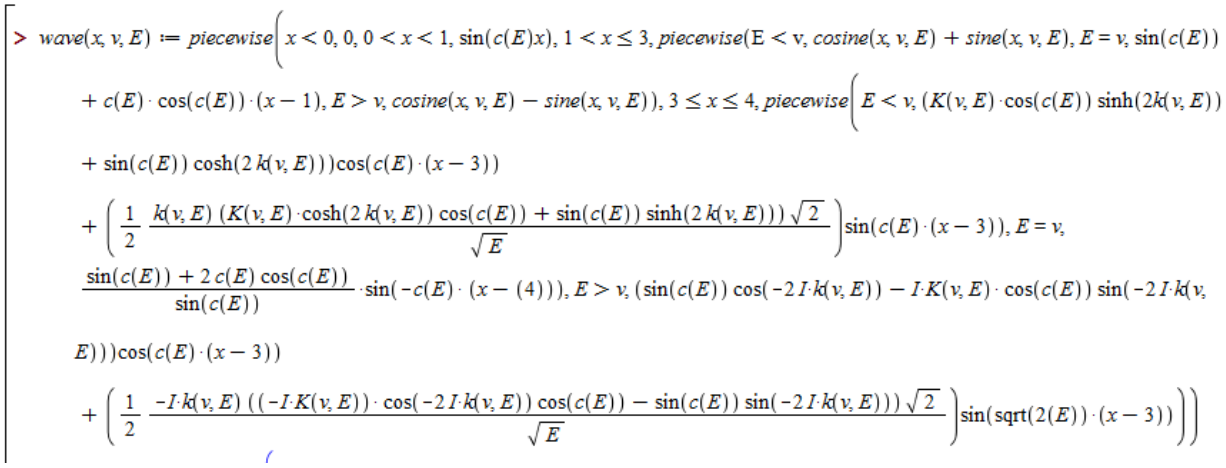

Figure 19: *Code for Double Well.*

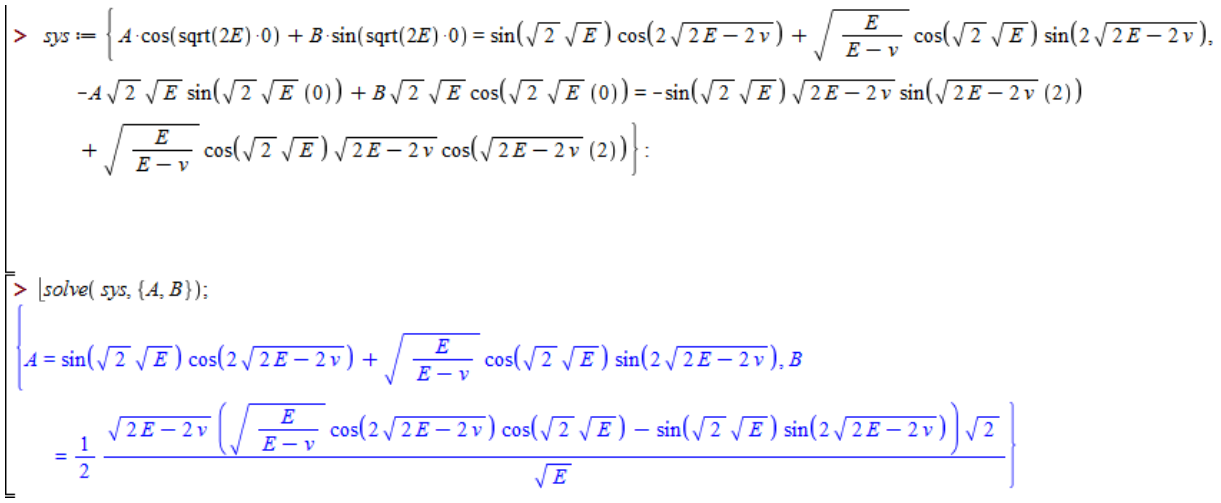

Figure 20: *Code for simultaneously solving for the coefficients of* $Acoskx + Bsinkx$ *in the double well region* $3 \leq x \leq 4$.

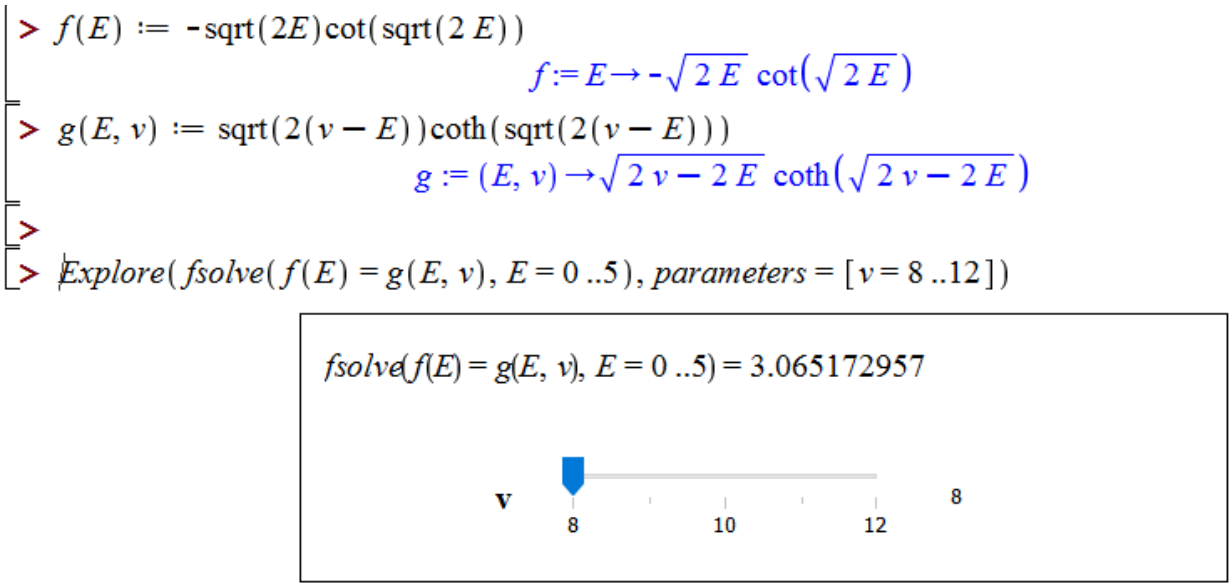

Figure 21: *Energy levels for asymmetric double well.*

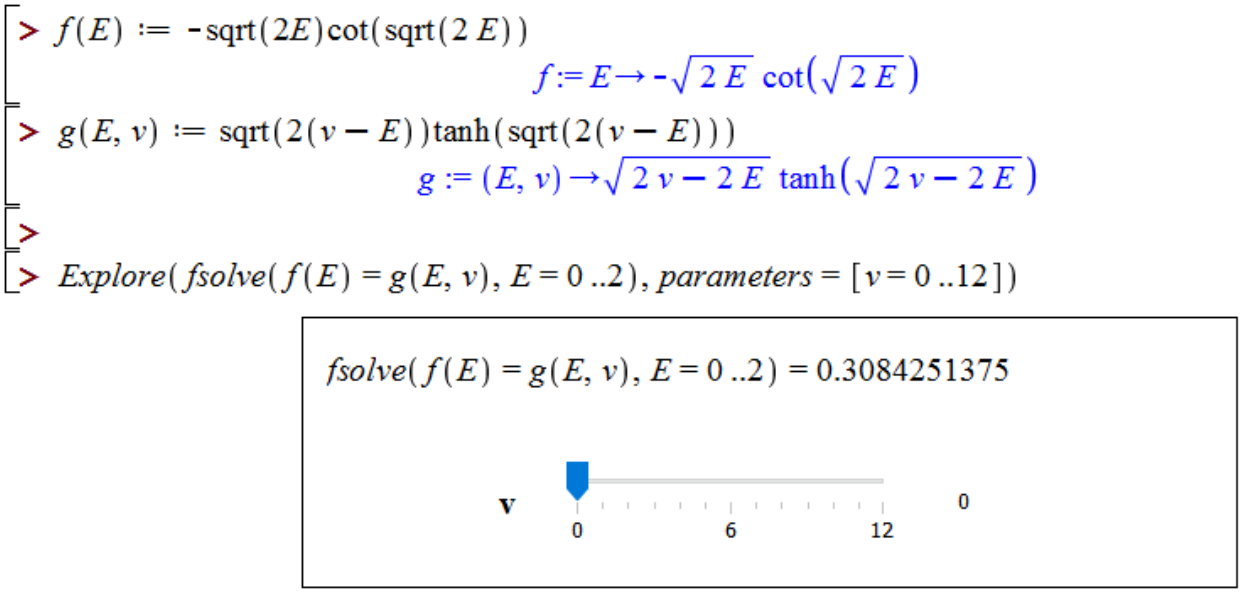

Figure 22: *Energy levels for symmetric double well.*

```
> for n from 2 to N do # Solves for coefficients and then populates wave array with complete wave functions
      wave_arr[1] := unapply(A[1]cos(k[1]·(x − a[1])) + B[1]sin(k[1]·(x − a[1])), x, E1, E2);

      k[n − 1] := sqrt(2 (m·(E1 + E2) − m·V[n − 1]));
      k[n] := sqrt(2 ( m·(E1 + E2) − m·V[n]));
      L[n − 1] := a[n] - a[n − 1];
      M := [ cos(k[n − 1]·L[n − 1])                    sin(k[n − 1]·L[n − 1])
             −(k[n − 1]/k[n])·sin(k[n − 1]·L[n − 1])    (k[n − 1]/k[n])·cos(k[n − 1]·L[n − 1]) ];
      AandB := M [ A[n − 1] ; B[n − 1] ];
      A[n] := AandB[1];
      B[n] := AandB[2];
      if V[n] < 20 then
          wave_arr[n] := unapply(A[n]cos(k[n]·(x − a[n])) + B[n]sin(k[n]·(x − a[n])), x, E1, E2);
      else
          wave_arr[n] := unapply(0, x, E1, E2);
      end if;
   if V[n] < Vmin then
   Vmin := V[n];
   end if
   end
>
```

Figure 23: *Code for the Nsteps simulations loop*

```
>
> f(E, v) := sqrt((2·0.1·(v − E))/1^2)·tan(3·sqrt((2·0.1·E)/1^2))
                  f := (E, v) → sqrt(2·0.1 (v − E)) tan(3 sqrt(2·0.1 E))
> g(E, v) := −sqrt((2·0.1·E)/1^2)·tanh(sqrt((2·0.1·(v − E))/1^2)·4)
                  g := (E, v) → −sqrt(2·0.1 E) tanh(4 sqrt(2·0.1 (v − E)))
>
> Explore(fsolve(f(E, v) = g(E, v), E = 0 ..8), parameters = [v = 5 ..15])
```

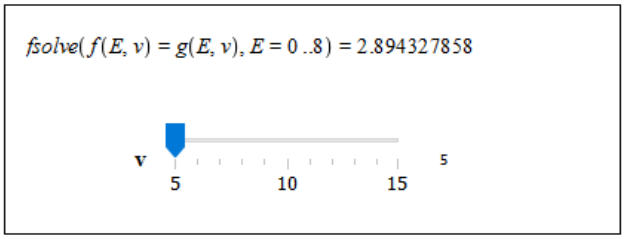

Figure 24: *Using Maple to find theoretical values E^t for well with finite step by using Eq.*(22) *and Eq.*(25)

V	E^e_{sym}	E^e_{asym}	E^t_{sym}	E^t_{asym}
6	4.62	5.67	4.73	5.39
7	5.03	6.02	5.16	5.67
8	5.40	6.28	5.53	5.91
9	5.70	6.37	5.85	6.13
10	6.00	6.49	6.12	6.34
11	6.25	6.69	6.36	6.52
12	6.45	6.81	6.57	6.69
13	6.66	6.98	6.75	6.85

Table 2: *A table to show experimental and theoretical Energy levels for different sized potential steps in an infinite double well*

Calendar of minutes

08/10/2016 - met with john at the library, we discussed aims of the project and briefly discussed what is expected of me throughout the year. We then decided I should do some reading on quantum mechanics and familiarise myself with maple before our next meeting after the weekend on Monday.

10/10/2016- John set me the task of checking to see if it was feasible to create the simulations in Matlab by attempting to design a simple single infinite well simulation. We also decided I should find double well solutions and try to design the simulation in Matlab or Maple. Finally we discussed the final aim of the project and both decided I should add a single harmonic oscillator simulation and create one simulation where x amount of finite steps can be added to the well with solutions.

17/10/2016- John used the Matlab simulation and we both agreed that the best course of action would be to make the simulations in maple as the UI would be much more suited to our needs. For this week we decided I would recreate the infinite well with a finite step in maple but this time use the EXPLORE functionality instead of ANIMATE.

24/10/2016- I showed John that I managed to make the well using the EXPLORE command. We decided I should be set the task of creating a double well simulation and find out how to use maple to solve differential equations.

31/10/2016- I showed John my double well simulation and also displayed a maple worksheet which solved the schrodinger equation for an infinite well, Then it was decided that I should find the values for the energy level in the finite and infinite well graphically. Also if possible, I would then add a functionality to the simulations which sets the wave functions equal to the energy level.

07/11/2016- John saw the solutions and suggested a change we could make to the double well simulations, where I match the wave function on the right to the boundary on the left to it, so that the wave function is continuous throughout the well. I also will make more changes so it is easier to use.

14/11/2016- After matching the wave differently I showed John that the wave in the right well for when E is larger than V was incorrect even as the differentials of the wave functions did not match. So John gave me guidance on how to fix the wave. He also suggested I plotted the energy levels on the graph.

21/11/2016- I showed John the fixed wave function and he noticed the wave was slightly incorrect when E is smaller than V so I was set to fix that. Also the method I used to plot the energy levels broke down in some cases, so John suggested I try to use a lookup table.

28/11/2016- After attempting to fix the wave again, it was still incorrect. I also showed John the new simulation I made with two potential barriers, he suggested I begin work on a simulation that displays n adjustable potential barriers. He also found that in maple, and imaginary cosine will become a hyperbolic cosine function.

5/12/2016- The double well was finally fixed and ready for John to use in his lectures, however we decided there were changes to be made for the two step functions and that I should write some pseudocode for the n-step well.

9/01/2017- I discussed with John that there would be issues and limitations to the n-steps well. We decided we wouldn't meet the week after due to exams and that I would attempt to make progress with the n-step well

23/01/2017- John showed me that the imaginary coefficient for the sinh function would cancel the imaginary root, and so we wouldn't have an exponential amount of wave functions so the n-step well is possible.

31/01/2017- The loop based on using maples simultaneous equation solving function would not work well so we decided I would instead find a recurrence relation in matrix form and instead attempt to incorporate this into the loop.

8/02/2017- In the meeting we discussed the matrix but as it was hard to understand, we came up with the idea that I should write a short article on how to find the wave function for each step.

15/02/2017- After handing John the article, he decided that we should use the matrix transfer method. We spent the meeting discussing what this is and how to apply it to my simulation for N steps.

22/02/2017- I showed John my N steps simulations where it was not user-friendly but all the maths was correct and the loops were functioning. We agreed I was to spend the next week figuring how to make the simulation user-friendly

01/03/2017- John made some suggestions of things that should be added to the simulation. Such as a method of choosing pre-set wells and to add mass to the equations

08/03/2017- After showing John the updated simulation, we thought it would be a good idea to make a course and fine method of changing the energy, on top of this it was suggested that I should make a problem sheet to compliment the use of the well.

15/03/2017- I showed John an improved version of the well which was much more user friendly, and I also created a problem sheet that would fully utilise the simulation. It was then decided I'd make a few more changes and get a friend to test the simulation.

22/03/2017- In this meeting, it was decided that I was to finalise the simulations and create a plan for the report.

29/03/2017- After showing the report plan to John, and making a few slight modifications to it, we planned that I was to finish a 1st draft for the report by 3rd May.

Physics Department
General Risk Assessment Form

(Refer to Notes for Guidance before completing this form)

Dept. Assessment No.	
Title of Activity:	Theoretical Project Work
Location(s) of Work:	N/A

Brief Description of Work: Please put here the title of your theoretical project or thesis

Quantum simulations

Hazard Identification: Identify all the hazards; evaluate the risks (low / medium / high); describe all existing control measures and identify any further measures required. Specific hazards should be assessed on a separate risk assessment form and cross-referenced with this document. Specific assessments are available for hazardous substances, biological agents, display screen equipment, manual handling operations and fieldwork.

Hazard (s)	**Risk** L / M / H	**Control Measures** (i.e., alternative work methods / mechanical aids / engineering controls, etc.)
Repetitive strain injury due to prolonged time using a keyboard and mouse.	L	Assess working position and provide wrist /hand support as appropriate. Take regular breaks away from work station.
Eye strain due to prolonged time looking at monitor.	L	Make sure seating position and monitor height are suitable for vision and wear appropriate glasses if needed. Take regular breaks away from workstation.
Back / neck ache due to prolonged time at work station and or incorrect sitting position.	L	Take regular breaks away from the work station. If back or neck pain persists, arrange for a DSE assessment by DSE assessor and take appropriate action. Eg. Special chair and/ or desk.
Electrical shock risk.	L	Safety electrical check of computer and it's associated hardware.
Trip hazard around workstation area	L	Keep area around and on workstation clean and tidy, remove any trip hazards.

**Continue on separate sheet if necessary*

Engineering Controls: *Tick relevant boxes*

Guarding		Extraction (LEV)		Interlocks		Enclosure	
Other relevant information (incl. testing frequency if appropriate):							

Personal Protective Equipment (PPE): Identify all necessary PPE.

Eye / Face		Hand /Arm		Feet / Legs		Respiratory	
Body (clothing)		Hearing		Other (Specify)			
Specify the grade(s) of PPE to be worn:							
Specify when during the activity the item(s) of PPE must be worn:							

Non-disposable items of PPE must be inspected regularly and records retained for inspection

Persons at Risk: Identify all those who may be at risk.

Academic staff		Technical staff		P'Grad students		U'Grad students	x
Maintenance staff		Office staff		Cleaning staff		Emergency personnel	
Contractors		Visitors		Others			

Additional Information: Identify any additional information relevant to the activity, including supervision, training requirements, special emergency procedures, requirement for health surveillance etc.

Assessment carried out by:

Name:	Print	BEN WOODHOUSE	Sign		Date: 3/05/2017
Supervisor:	Print	J. SAMSON	Sign	J. Samson	Review Date: 3/5/2018

Supervisor must set up reminder for review date on their Outlook Calendar

Outlook reminder set up ✓

Quantum Mechanics: Simulation Problem Set

Ben Woodhouse & Dr John Samson

09/03/2017

Problem 1 *Well With Finite Step*

To create this specific type of well, select the 'step' button and then executing the whole worksheet (the three exclamation marks on the tool-bar). Start with the mass, m set to 0.1 by using the slider at the top of the page. When we start to increase the mass you may need to use $E2$ to fine tune a solution. the Energy of the wave function, E is given by $E = E1 + E2$.

1a) Find E and sketch the ground state for the step well when $m = 0.1$
1b) Comment on the wave function you can see. Explain how the wave behaves inside the well and below the potential barrier.
1c) How does this compare to classical physics?

2a)Find E and sketch the state $n = 2$ for when $m = 0.1$.
2b)Describe the shape of the wave function and Explain why it behaves this way.
2c) Set $m = 0.3$ and Sketch the new wave function for the state of $n = 2$. Compare this to the sketch in 2a).

Problem 2 *Double Well*

To create a Double well, Click the 'Double' button and then execute the worksheet.

1a) Set $m = 0.4$ and find E for the symmetric and anti-symmetric wave functions for the state $n = 2$. Sketch the wave functions.
1b) Explain the wave function across both wells and the potential barrier for $n = 2$.
1c) Find E for the symmetric wave function for the state $n = 3$. Sketch the wave function and compare this to the symmetric wave function at $n = 2$.

Problem 3 *Custom Well*

To create a Custom well, edit the array named 'V_CUSTOM', press the 'Custom' button and then execute the worksheet. (the first value must be kept as 0)

1. Create an infinite well (infinite barrier has a value of 20) and sketch the first 4 Energy Eigenstates when $m = 0.5$.

2. Create a well with the array $[0, 1, 2, 3, 4, 5, 6, 20]$ and sketch the state $n = 4$ when $m = 1.0$. Explain what is happening to the wave function here.

3. Create a well with the array $[0, 10, 10, 0, 10, 10, 0, 20]$ and a wave function with $m = 1.0$. Find the state $n = 2$ and describe what you can see here.