Computational Physics Case Study 2: Numerical Solutions of Schrodinger's Equation

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1   Introduction

There are relatively few analytic solutions to Schrodinger's equation so it is often necessary to seek a numerical solution in order to be able to model various quantum systems. In this project, we will use two methods suited to boundary value problems, the first being numerical integration and the second being matrix evaluation. They are first employed in order to solve Schrodinger's equation for the one-dimensional infinite potential, then they are used to further study the case of a linear potential, and various situations such as the double square well (quadratic and quartic) potentials. Later in the project, time dependence for a superposition of stationary states is also studied, for the case of an ammonia molecule, using the matrix approach.

2   Theory

The one dimensional, time independent, Schrodinger equation (TISE) is

$$\hat{H}\psi = E\psi \Rightarrow \Big[-\frac{\hbar^2}{2m}\frac{d^2}{dx} + V(x)\Big]\psi = E\psi \tag{1}$$

Here the potential V(x) is a function of position only, so the Hamiltonian operator $\hat{H}$ is independent of time. The TISE is an energy eigenvalue equation, and the eigenvalues E_n (allowed energies), and corresponding eigenfunctions $\psi_n(x)$ (probability amplitudes) of the bound states, need to be determined for a given potential V(x). In this case a general time dependent solution can then be represented as a superposition of the eigenstates of $\hat{H}$:

$$\Psi(x,t) = \sum_n a_n\psi_n\exp\Big(-\frac{iE_nt}{\hbar}\Big) \tag{2}$$

Acceptable bound state solutions are quantised, hence the summation over n. The $\psi_n(x)$ must be normalizable, i.e. for finite V(x) we require that $\psi_n(x)$ and $\frac{d\psi_n}{dx}$ be continuous, finite and single-valued for all x. [2]

The TISE is a second-order differential equation so two boundary conditions are generally required to uniquely determine a solution. For a symmetric potential, $V(x) = -V(x)$, a definite parity is imposed on $\psi_n(x)$. Even parity solutions have $\psi_n(-x) = \psi_n(x)$, while odd parity solutions have $\psi_n(-x) = -\psi_n(x)$. This definite parity allows us to specify either $\psi_n(x)$ or $\frac{d\psi_n(x)}{dx}$ at x=0.

3 Procedures

3.1 The shooting method

3.1.1 Background

The shooting method is possibly the simplest approach to numerical integration of the TISE, and it exploits the fact that the equation is linear in ψ. The approach can be broken down into a number of steps.

First the range of x is divided into N intervals of width Δx and a suitable notation for a numerical integration is adopted. Second V(x) is defined and values of ψ, $\dfrac{d\psi}{dx}$ are specified for an initial position. For odd parity solutions $\psi(0) = 1$, $\psi'(0) = 0$. For even parity solutions $\psi(0) = 0$, $\psi'(0) = 1$. The non-zero value of ψ, ψ' is arbitrary. Then a trial guess at an energy eigenvalue E is made, based on physical intuition.

At this point, the TISE can be integrated from the initial position to some suitable final position, using one of Matlabs standard ODE integrators. A check is then performed to see if the solution for ψ has satisfied the boundary conditions of the problem. This is unlikely to be the case at the first trial, so the energy eigenvalue is then adjusted, the numerical integration is repeated, and a check is again performed to see if the boundary conditions are satisfied. This trial and error stage typically involves several iterations. When the boundary conditions are satisfied to reasonable accuracy, the eigenfunction is normalised and then plotted along with the eigenvalue.

This approach is applied to the particle in a box (infinite potential well) problem. For this problem, any solution must have $\psi_n = 0$ at the edges of the box $(x = 0, L)$, where the potential is infinite. Starting values for ψ, $\dfrac{d\psi}{dx}$ are provided at the left hand edge of the box $(x = 0 \to \psi = 0, \dfrac{d\psi}{dx} = 1)$. Using the initial data, a numerical step-by-step integration of the TISE is used to solve for $\psi(x)$ between $x = 0$ and $x = L$. The required boundary condition at the right hand edge of the box is $\psi = 0$, and this value is set to be achieved by suitably adjusting E.

In order to numerically integrate the TISE, it can be written in the form

$$\frac{d^2\psi}{dx^2} = \frac{2m}{\hbar^2}(V(x) - E)\psi, \quad 0 < x < L \tag{3}$$

Here a certain set of units is employed, in order to avoid very small or very large numbers appearing in the equations to be solved:

$$\begin{cases} 1\,\text{Å} = 10^{-10}\text{m} \\ 1\text{m}_\text{e} = 9.1094 \times 10^{-31}\text{kg} \\ 1\text{eV} = 1.6022 \times 10^{-19}\text{J} \\ \hbar = 1.0546 \times 10^{-34}\text{J s} \end{cases}$$

The box potential is zero in the interior, and infinite at the edges. A box with width $L = 1$ nm $=$ 10 Angstrom is chosen and the particle in the box is assumed to be an electron, i.e. $m = 1$. For numerical integration, Matlab's *ode45* is employed, and the corresponding modified script-files (*shoot1studentV, shoot1student*) are supplied in Appendix 1.

3.1.2   Analysis and results

Indeed by adopting the set of units and constants listed in Section 3.1.1, and plugging them into Eq. 3, converting into the adopted units (energy in eV, length in Angstroms and mass in electron masses), the TISE can then be re-written as

$$\frac{d^2\psi}{dx^2} = 0.26246m(V(x) - E)\psi \tag{4}$$

Using Eq. 4 and the script-file *shoot1student*, the first 4 eigenvalues for the 1-D box were calculated, correct to 3 decimal places. They are in very good agreement with the well-known analytic solutions obtained from Eq. 5:

$$E_n = \frac{n^2\pi^2\hbar^2}{2ma^2} \tag{5}$$

$$\begin{cases} E_1 = 0.376 \text{ eV} \\ E_2 = 1.504 \text{ eV} \\ E_3 = 3.384 \text{ eV} \\ E_4 = 6.017 \text{ eV} \end{cases}$$

The resulting eigenfunctions and probability densities shifted at the same level are presented in Fig. 1.
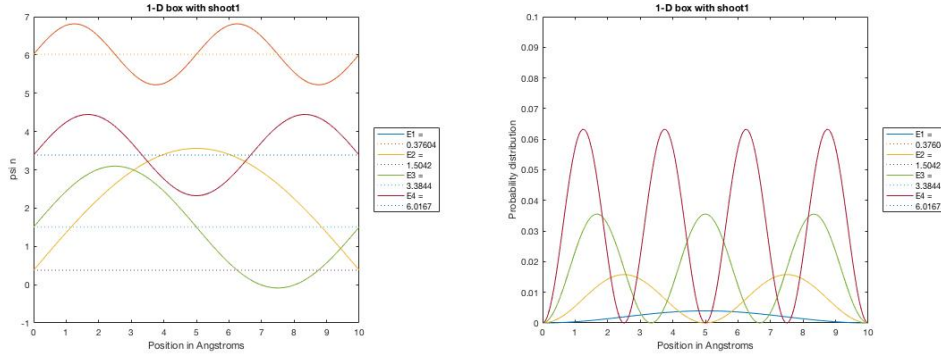

Figure 1: Eigenfunctions (a) and probability densities (b) of the first 4 energy states for a 1-D box

The case of an electron bound in a linear potential is then considered, with the obvious starting point for integration x = 0. In this situation, the potential V(x) is given by

$$V(x) = \begin{cases} \infty & x \leq 0 \\ \alpha x & x > 0 \end{cases} \quad \text{with} \quad \alpha = 1\,\text{eVÅ}^{-1}, \quad m = 1 \tag{6}$$

The eigenvalues and eigenfunctions for the first 3 energy states are presented in Fig. 2. The eigenvalues, listed below, are in quite good agreement with the results from the analytical solution, being slightly less than the values derived from Eq. 7. [1]
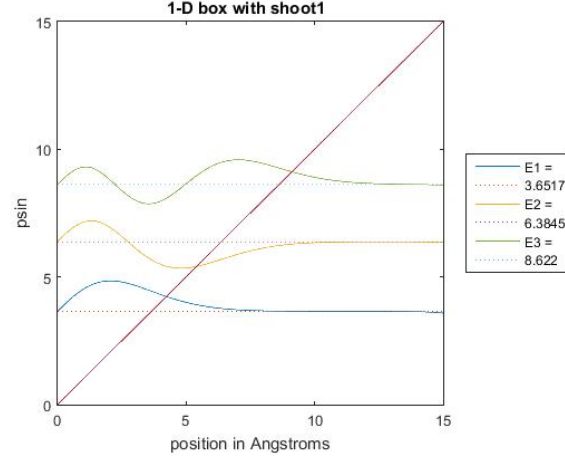
Figure 2: Eigenfunctions and corresponding eigenvalues of the first 3 energy states for the linear potential

$$\begin{cases} E_1 = 3.6517 \text{ eV} \\ E_2 = 6.3845 \text{ eV} \\ E_3 = 8.622 \text{ eV} \end{cases}$$

$$\frac{E_n}{(m\hbar^2 g^2/2)^{1/3}} = [3\pi(n-1/4)/2]^{2/3} \quad \text{where} \quad mg^2 = \frac{\alpha^2}{m} \tag{7}$$

A potential of this form (i.e. V(x)) can, for instance, model a ball which bounces vertically on a rigid horizontal plane, in a macroscopic setting, or a particle falling under gravity in a microscopic setting. In both cases $\alpha = mg$. While at the quantum stage the energy levels are the ones presented in Fig. 2, in the classical limit (n very large) the discrete levels are so densely packed that they approximate to a continuum. Another example of a linear potential could be an electron placed in a constant electric field of a thin capacitor. In this case $V = -qEx$ between the plates of the capacitor. Here α is the negative of the electric force i.e. $\alpha = -qE$.

3.2 Matrix approach

3.2.1 Background

The TISE is a separable solution of Schrodinger's equation:

$$i\hbar\frac{\partial}{\partial t}|\psi\rangle = \hat{H}|\psi\rangle \tag{8}$$

where

$$|\psi(x,t)\rangle = |\psi(x)\rangle\, e^{-\frac{iEt}{\hbar}} \tag{9}$$

and

$$\hat{H}|\psi(x)\rangle = E|\psi(x)\rangle \tag{10}$$

The finite difference method is a common numerical approach to solving a partial differential equation such as the 1-D TISE. The approach for a 1-D problem is to sample functions at a set of equally spaced points, so that the position variable is,

$$x_j = j \times s, \quad j \in \mathbb{N} \tag{11}$$

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where s is the length of the step, i.e. $x_{j+1} = x_j + s$. The difference approximations for the derivatives of the wave function are then defined as

$$
\begin{cases}
\dfrac{d}{dx}\psi(x_j) = \dfrac{\psi(x_j) - \psi(x_{j-1})}{s} \\
\dfrac{d^2}{dx^2}\psi(x_j) = \dfrac{\psi(x_{j-1}) - 2\psi(x_j) + \psi(x_{j+1})}{s^2}
\end{cases}
\tag{12}
$$

By substituting into the TISE, $\hat{H}\psi = \left[-\dfrac{\hbar^2}{2m}\dfrac{d^2}{dx} + V(x) \right]\psi = E\psi$, Eq. 12 can be re-expressed in the matrix form as

$$
\begin{cases}
(\hat{H} - E\hat{I})\psi(x) = \displaystyle\sum_{j=0}^{N} \left(-u\psi(x_{j-1}) + (d_j - E)\psi(x_j) - u\psi(x_{j+1}) \right) = 0 \\
d_j = \dfrac{\hbar^2}{ms^2} + V_j, \quad u = \dfrac{\hbar^2}{2ms^2}
\end{cases}
\tag{13}
$$

For the 1-D box problem, suitable boundary conditions are $\psi(x_0) = \psi(x_N) = 0$, so that in this case the matrix equation becomes

$$
(\hat{H} - E\hat{I})\psi =
\begin{bmatrix}
(d_1 - E) & -u & 0 & 0 & \cdot & & \cdot \\
-u & (d_2 - E) & -u & 0 & \cdot & & \cdot \\
0 & -u & (d_3 - E) & -u & \cdot & & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & & \cdot \\
\cdot & \cdot & \cdot & \cdot & \cdot & & \cdot \\
\cdot & \cdot & \cdot & \cdot & -u & (d_{N-1} - E)
\end{bmatrix}
\begin{bmatrix}
\psi_1 \\ \psi_2 \\ \psi_3 \\ \cdot \\ \cdot \\ \psi_{N-1}
\end{bmatrix}
= 0
\tag{14}
$$

A script file in Matlab ($tqm4$) is used to solve Eq. 10 through the matrix approach for the lowest eigenfunctions and eigenvectors, given a one-dimensional time independent potential, specified analytically as a function of x.

3.2.2 Analysis and results

The script file is first adapted for the double well square potential to investigate how the eigenfunctions and eigenvalues change if the width of the central barrier is increased. Tunneling from one state to the other can occur through the potential barrier. The ground state configuration has a symmetric and an anti-symmetric solution with slightly differing energies, as can be seen in Fig. 3 below.
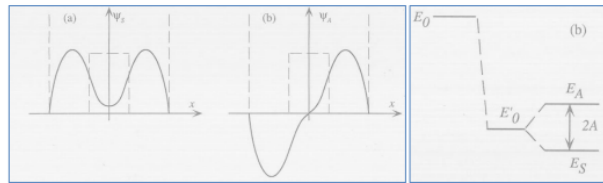

Figure 3: The ground state configuration for the ammonia molecule

The particles are, for a time, confined however there is always a non-zero tunneling probability and therefore it cannot be said with certainty that the particles remain on one side or the other of the potential barrier. The important point here is that there are two almost degenerate energy

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eigenstates for every one energy eigenstate in the corresponding finite square well. If the width of the barrier is made even greater, then the ground state energy would approach that of the finite square well and the splitting between the energy levels would be even smaller, as can be seen in Fig. 4. This is because for a large enough barrier width, each well will approximate a finite 1-D box.
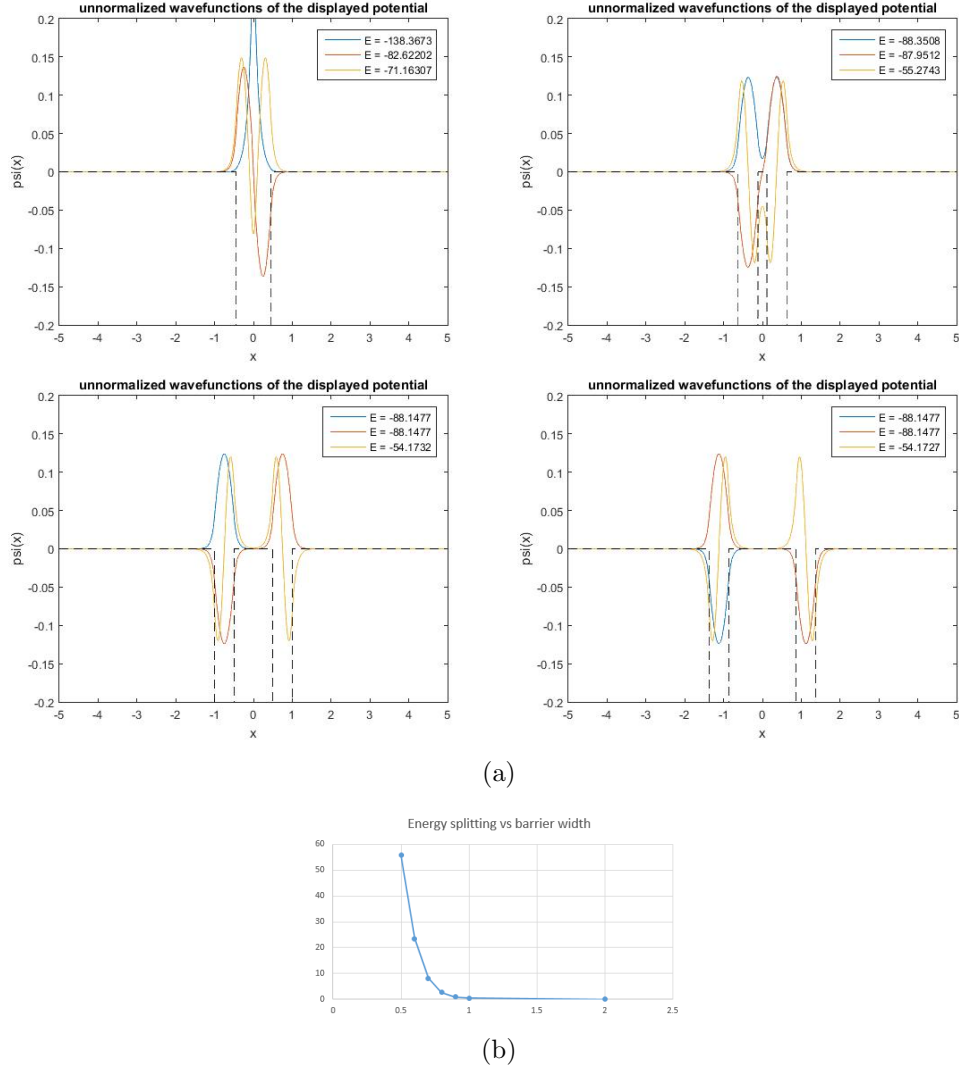

(a)

(b)

Figure 4: (a) Ground state energy eigenstates for the finite double well potential at barrier widths of 0.5, 1, 2 and 3 times the default value (b) The coupling of the ground states (difference in eV) as a function of well spacing

Next, the quartic double well potential is analyzed. Its expression is given by

$$V(x) = \frac{V_{max}}{b^4} \left[\left(x - \frac{a}{2} \right)^2 - b^2 \right]^2 - V_0 \tag{15}$$

with the well minima located at $\frac{a}{2} \pm b$, $V_{max} = 10$, $V_0 = 100$, $a = 0$, $b = 1.5$.

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The eigenvalues are $E_S = -97.1444$ eV for the symmetric solution, $E_A = -97.1387$ eV for the anti-symmetric solution, and the eigenfunctions for the ground state are presented in Fig. 5.
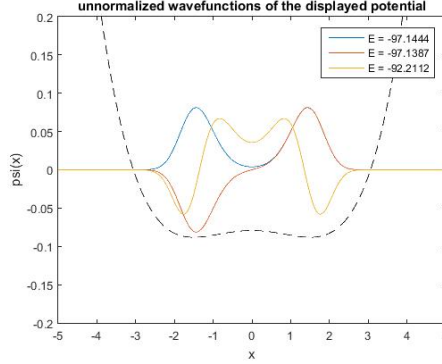

Figure 5: Eigenfunctions for the ground state of the quartic double well potential

3.3 Time dependence

3.3.1 Background

From Eq. 2 in Section 2 we know that a superposition of stationary states will exhibit time dependence. When the symmetric (S) and anti-symmetric (A) ground states are superposed we can expect time dependent behaviour and this is displayed using a script file in Matlab (*tqm5*). In nature this behaviour is mirrored by, for example, the ammonia molecule.

Considering the ground state wave function $\psi(x,t)$ to equal ψ_R at time $t = 0$. Its time evolution is:

$$\psi(x,t) = \frac{1}{\sqrt{2}}\left(\psi_S(x)\exp\left(-\frac{iE_S t}{\hbar}\right) + \psi_A(x)\exp\left(-\frac{iE_A t}{\hbar}\right)\right) \tag{16}$$

or

$$\psi(x,t) = \frac{\exp\left(-\frac{iE_S t}{\hbar}\right)}{\sqrt{2}}\left(\psi_S(x) + \psi_A(x)\exp(-i\omega t)\right) \tag{17}$$

where we have introduced the Bohr frequency given by $\hbar\omega = E_A - E_S$. [3]

For the superposition $\Psi = c_1\psi_1 + c_2\psi_2$ where c_1, c_2 are complex in general, the time dependent probability density becomes:

$$|\Psi(x,t)|^2 = |c_1|^2|\psi_1(x)|^2 + |c_2|^2|\psi_2(x)|^2 + 2\Re(c_1^* c_2 \psi_1^*(x)\psi_2(x)) \tag{18}$$

This is illustrated for a particle trapped in a double well potential by choosing an equally weighted superposition of the ground and first excited states, with the particle initially located in the right hand well.

3.3.2 Analysis and results

Indeed we can derive Eq. 18 by using that

$$|\Psi(x,t)|^2 = \Psi\Psi^* = (c_1\psi_1 + c_2\psi_2)(c_1^*\psi_1^* + c_2^*\psi_2^*) = |c_1|^2|\psi_1(x)|^2 + |c_2|^2|\psi_2(x)|^2 + c_1 c_2^*\psi_1\psi_2^* + c_2 c_1^*\psi_2\psi_1^*$$

Now by using that $\Re(z) = \frac{z + z^*}{2}$, it follows that

$$2\Re(c_1^* c_2 \psi_1^*(x)\psi_2(x)) = c_1 c_2^*\psi_1\psi_2^* + c_2 c_1^*\psi_2\psi_1^* \tag{19}$$

so by substituting back into the expression for $|\Psi(x,t)|^2$, we get Eq. 18.

We then adapt this to the case when $c_1 = c_2 = \frac{1}{\sqrt{2}}$ and $\psi_1, \psi_2 \in \mathbb{R}$ in order to determine the angular frequency. In this case

$$
\begin{cases}
\psi_1(x) = \phi_1 e^{-\frac{iE_1 t}{\hbar}} \Rightarrow \psi_1^*(x) = \phi_1 e^{+\frac{iE_1 t}{\hbar}} \\
\psi_2(x) = \phi_2 e^{-\frac{iE_2 t}{\hbar}}
\end{cases}
\tag{20}
$$

Equation 18 can now be re-written as

$|\Psi(x,t)|^2 = \frac{1}{2}(\psi_1^2 + \psi_2^2) + \psi_1^* \psi_2 \Rightarrow |\Psi(x,t)|^2 = \frac{1}{2}(\psi_1^2 + \psi_2^2) + \phi_1\phi_2 e^{-\frac{i(E_2 - E_1)t}{\hbar}}$. So $\omega = \frac{E_2 - E_1}{\hbar}$. This is the same result that would be derived by re-writing Eq. 16 in the form of Eq. 17.

Finally, the time dependence of a two-state superposition in the double well potential is examined. The superposition in Eq. 16 represents a state that oscillates from right to left and back again. This is illustrated in the script file *tqm5* and in the Figure 6 below, in this case with a real example, the ammonia molecule, which in its ground state performs this periodic quantum tunneling in an oscillation between the odd and even states with angular frequency ω.
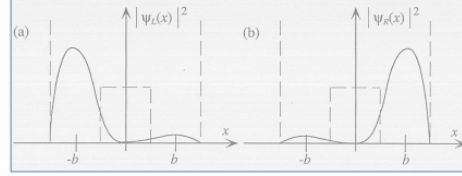

Figure 6: Time dependence of a two-state superposition in the double well potential

The time dependence of the superposition is determined by Equation 17. After a time $T = \pi\hbar/(E_A - E_S)$ the exponential in the brackets in Eq. 17 equals $e^{-\pi i} = -1$, so in an overall phase factor the wavefunction has become $[\psi_S(x)\psi_A(x)]/\sqrt{2}$, meaning that the particle is certainly in the left-hand well i.e. in the interval T the particle has tunneled through the barrier between the wells. After a further period T it is certainly in the right-hand well, and the process repeats as seen in Fig. 6.

We also examined the variation of time dependence with the depth, width and spacing of the wells, and the results are presented in Fig. 7.
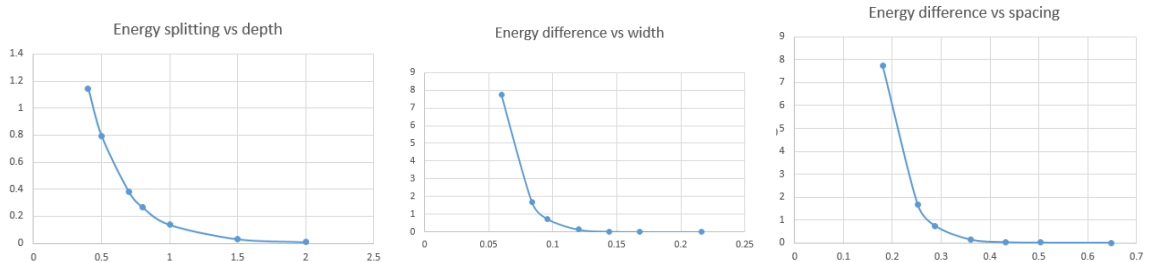

Figure 7: Evolution of time dependence with the depth, width and spacing of the wells. Time dependence is expressed in the form of the energy difference in eV between the anti-symmetric and symmetric states, which in this case is easily linked to the Bohr frequency since $\hbar = 1$ as it is normalized. All x-axis units are the default units used in the script file

The results in Fig. 7 indicate that as any of the parameters width, depth and spacing increases, the energy difference between the symmetric and anti-symmetric states drops exponentially. This is expected as any large enough increase in the above mentioned parameters brings the energy states of the system closer to those of two separate finite square wells.

4   Summary

From the results in this report we can conclude that both the numerical integration through the shooting method and the matrix approach are two very suitable ways in which Schrodinger's equation can be numerically solved. Using these two methods various systems with different potentials were accurately modeled and described. In addition to this, the relative convenience of modifying various parameters before the numerical calculation through the script has made easier to study and visualize the way systems change or evolve under certain circumstances.

References

[1] P.C.W.Davies and D.S.Betts, *Quantum Mechanics*, 2nd edition, Chapter 2

[2] A.I.M. Rae, *Quantum Mechanics*, 4th edition, Chapter 2

[3] Binney and Skinner, *The Physics of Quantum Mechanics*, OUP, Chapter 5

Appendix 1

- *shoot1student (adapted for probability densitites)*

```matlab
% -----------------------------------------------------
% Implements the shooting method to solve the TISE
% for a particle moving in a 1-D box with V(x) = 0
% inside domain [0,L] and V(x) infinite elsewhere.
% Atomic units are used.
% Length unit = 1 Angstrom 10^(-10) m
% Mass unit = 1 me (9.1094 x 10^(-31) kg)
% Energy unit = 1 eV (1.6022 x 10^(-19) J)
% In these units the TISE takes the form
% d2u/dx^2 = A*m*(V(x) - E)*u
% Boundary conditions at x = 0 are u = 0, du/dx = 1
% The TISE is written as two 1st order ODE's
% It is integrated using the Matlab solver ode45
% Anonymous function 'rhs' defines the 1sr order DE's
% The unnormalized wavefunction is plotted.
% The trial eigenvalue is set in script
%-----------------------------------------------------
% initial conditions and x range
y0 = [0 1];
xmax = 10;
dx = 0.01;
x = 0:dx:xmax;
% equation parameters
A = 0.26246;
m = 1;
V = 0;
% trial energy eigenvalue for n=1
E_value = 0.37604;
% 1st order representation of the TISE
rhs = @(x,y) [y(2); A*m*(V - E_value).*y(1)];
% call DE solver
[x,y] = ode45(rhs,x,y0);
% normalize solution for u
s = sum(y(:,1).^2);
total = s*dx;
u = y(:,1)/total;
% plot wave function
%plot(x,y(:,1) + E_value);
%hold on;
% plot prob. density
p_d=abs(u).^2;
plot(x,p_d);
hold on;
%plot energy level n=1
E_value1=E_value;
x1=[0 xmax];e1=[E_value1 E_value1];
plot(x1,e1,':');
hold on;
% trial energy eigenvalue for n=2
E_value = 1.504176;
% 1st order representation of the TISE
rhs = @(x,y) [y(2); A*m*(V - E_value).*y(1)];
% call DE solver
[x,y] = ode45(rhs,x,y0);
% normalize solution for u
```

```matlab
s = sum(y(:,1).^2);
total = s*dx;
u = y(:,1)/total;
% plot wave function
%plot(x,y(:,1) + E_value);
%hold on;
% plot prob. density
p_d=abs(u).^2;
plot(x,p_d);
hold on;
%plot energy level n=2
E_value2=E_value;
x1=[0 xmax];e1=[E_value2 E_value2];
plot(x1,e1,':');
hold on;
% trial energy eigenvalue for n=3
E_value = 3.38439;
% 1st order representation of the TISE
rhs = @(x,y) [y(2); A*m*(V - E_value).*y(1)];
% call DE solver
[x,y] = ode45(rhs,x,y0);
% normalize solution for u
s = sum(y(:,1).^2);
total = s*dx;
u = y(:,1)/total;
% plot wave function
%plot(x,y(:,1) + E_value);
%hold on;
% plot prob. density
p_d=abs(u).^2;
plot(x,p_d);
hold on;
%plot energy level n=3
E_value3=E_value;
x3=[0 xmax];e3=[E_value3 E_value3];
plot(x3,e3,':');
hold on;
% trial energy eigenvalue for n=4
E_value = 6.016705;
% 1st order representation of the TISE
rhs = @(x,y) [y(2); A*m*(V - E_value).*y(1)];
% call DE solver
[x,y] = ode45(rhs,x,y0);
% normalize solution for u
s = sum(y(:,1).^2);
total = s*dx;
u = y(:,1)/total;
% plot wave function
%plot(x,y(:,1) + E_value);
%hold on;
% plot prob. density
p_d=abs(u).^2;
plot(x,p_d);
hold on;
%plot energy level n=4
E_value4=E_value;
x4=[0 xmax];e4=[E_value4 E_value4];
plot(x4,e4,':');
hold on;
%plot labelling
xlabel('Position in Angstroms');
```

```matlab
ylabel('Probability distribution');
%ylabel('psi n');
ttl=['1-D box with shoot1  ']%,...
    %'E1 = ',num2str(E_value1)];
title(ttl);
%axis([0 10 0 0.1])
legend('E1 = ',num2str(E_value1),'E2 = ',num2str(E_value2),'E3 =
',num2str(E_value3),'E4 = ',num2str(E_value4),'location','eastoutside')
```

- ***shoot1student_V***

```matlab
% -------------------------------------------------
% Implements the shooting method to solve the TISE
% for a particle moving in a 1-D box with V(x) = 0
% inside domain [0,L] and V(x) infinite elsewhere.
% Atomic units are used.
% Length unit = 1 Angstrom 10^(-10) m
% Mass unit = 1 me (9.1094 x 10^(-31) kg)
% Energy unit = 1 eV (1.6022 x 10^(-19) J)
% In these units the TISE takes the form
% d2u/dx^2 = A*m*(V(x) - E)*u
% Boundary conditions at x = 0 are u = 0, du/dx = 1
% The TISE is written as two 1st order ODE's
% It is integrated using the Matlab solver ode45
% Anonymous function 'rhs' defines the 1sr order DE's
% The unnormalized wavefunction is plotted.
% The trial eigenvalue is set in script
%-------------------------------------------------
% initial conditions and x range
y0 = [0 1];
xmax = 15;
dx = 0.01;
x = 0:dx:xmax;
% equation parameters
A = 0.26246;
m = 1;
alpha = 1;
V = alpha*x;
% trial energy eigenvalue for n=1
E_value = 3.651677;
% 1st order representation of the TISE
rhs = @(x,y) [y(2); A*m*(alpha*x - E_value).*y(1)];
% call DE solver
[x,y] = ode45(rhs,x,y0);
% normalize solution for u
s = sum(y(:,1).^2);
total = s*dx;
u = y(:,1)/total;
% plot wave function
plot(x,y(:,1) + E_value);
hold on;
%plot energy level n=1
E_value1=E_value;
x1=[0 xmax];e1=[E_value1 E_value1];
plot(x1,e1,':');
hold on;
% trial energy eigenvalue for n=2
E_value = 6.38455;
```

```matlab
% 1st order representation of the TISE
rhs = @(x,y) [y(2); A*m*(alpha*x - E_value).*y(1)];
% call DE solver
[x,y] = ode45(rhs,x,y0);
% normalize solution for u
s = sum(y(:,1).^2);
total = s*dx;
u = y(:,1)/total;
% plot wave function
plot(x,y(:,1) + E_value);
hold on;
%plot energy level n=2
E_value2=E_value;
x1=[0 xmax];e1=[E_value2 E_value2];
plot(x1,e1,':');
hold on;
% trial energy eigenvalue for n=3
E_value = 8.622;
% 1st order representation of the TISE
rhs = @(x,y) [y(2); A*m*(alpha*x - E_value).*y(1)];
% call DE solver
[x,y] = ode45(rhs,x,y0);
% normalize solution for u
s = sum(y(:,1).^2);
total = s*dx;
u = y(:,1)/total;
% plot wave function
plot(x,y(:,1) + E_value);
hold on;
%plot energy level n=3
E_value3=E_value;
x3=[0 xmax];e3=[E_value3 E_value3];
plot(x3,e3,':');
hold on;
plot(x,V);
hold on;
%plot labelling
xlabel('position in Angstroms');
ylabel('psin');
ttl=['1-D box with shoot1  ']%,...
    %'E1 = ',num2str(E_value1)];
title(ttl);
legend('E1 = ',num2str(E_value1),'E2 = ',num2str(E_value2),'E3 =
',num2str(E_value3),'location','eastoutside')
```