The Numerical Solution of the Time-Independent 1-D Schrodinger Equation.

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1 Abstract

In this laboratory, I used the python language to solve the one dimensional time-independent Schrödinger equation numerically for an infinite square well potential both with and without a harmonic term. For computational purposes, I worked in a dimensionless regime with discretised position coordinates. The energy eigenvalues of each potential were found using the Numerov method which only returns values which satisfy the boundary conditions of the problem up to a specified accuracy. It was found that in the case of the regular infinite well, which is analytically solvable, the energies obtained using this method agreed precisely with the analytical solutions up to the order of the chosen value for accuracy, at higher orders the solutions began to differ. The Heisenberg uncertainty relation was shown to be satisfied for the first ten eigenstates of each potential, furthermore, the ground state solution in the harmonic potential had minimum uncertainty, suggesting that its analytical solution is a Gaussian wavepacket.

2 Introduction: Analytical Solutions and Non-Dimensionalisation

The time-independent Schrodinger equation for a particle described by the state $\psi(x)$ in an infinite, square well potential is

$$\frac{d^2\psi}{dx^2} + \frac{2mV_0}{\hbar^2}\psi\left(\frac{E}{V_0} - 1\right) = 0, \qquad V(x) = \begin{cases} V_0 & \text{if } 0 < x < L \\ +\infty & \text{if } elsewhere \end{cases}. \tag{2.1}$$

We can non-dimensionalise the equation (2.1) by rescaling the coordinate x as $\tilde{x} = x/L$ and then making the following definitions:

$$\gamma^2 = \frac{2mL^2V_0}{\hbar^2} \qquad \epsilon = \frac{E}{V_0} \qquad \nu(\tilde{x}) = \frac{V(\tilde{x})}{V_0}$$

Note that $\nu(\tilde{x}) \in [-1, +1]$. Then we obtain the dimensionless form of (2.1)

$$\frac{d^2\psi(\tilde{x})}{d\tilde{x}^2} + \gamma^2(\epsilon - \nu(\tilde{x}))\psi(\tilde{x}) = 0. \tag{2.2}$$

In the region where $0 < \tilde{x} < 1$ we set $\nu = -1$ then the general solution is $\psi(\tilde{x}) = A\sin(k\tilde{x}) + B\cos(k\tilde{x})$ where $k = \gamma\sqrt{\epsilon+1}$. Then we can use the condition that ψ must vanish at $\tilde{x} = 0, 1$ which implies $k = \pi n$ where $n = 0, 1, 2$. Thus we have the following solutions and their corresponding energies:

$$\psi_n(\tilde{x}) = A\sin(\pi n\tilde{x}) \qquad \epsilon_n = \frac{\pi^2(n+1)^2}{\gamma^2} - 1 \tag{2.3}$$

The uncertainty relation in terms of non-dimensional coordinates and momenta becomes $\Delta\tilde{x}\Delta\tilde{p} \geq 0.5$.

3 Methodology

To implement the Numerov method in python to find the energy eigenvalues of $\psi(\tilde{x})$, three starting values were chosen for the iterative process to update, $\psi(0) = 0$, $\psi(1) = 10^{-4}$, and a trial energy ϵ which must be below the eigenvalue of interest. We discretise the physical distance of the well into N=1000 points at which psi can be evaluated. The wave function for ϵ is approximated at the $(n+1)^{th}$ point in the system as

$$\psi_{n+1} = \frac{2(1 - \frac{5}{12}l^2k_n^2)\psi_n - (1 + \frac{1}{12}l^2k_{n-1}^2)\psi_{n-1}}{1 + \frac{1}{12}l^2k_{n+1}^2}, \quad where \quad l = \frac{1}{N-1}. \tag{3.1}$$

Then the code written to evaluate ψ at every point of the discretised distance is:

```
for x in range(1,N-1):
    psi[x+1] = (2*(1-(5/12)*(l**2)*(k2[x]))*(psi[x])
     - (1 + (1/12)*(l**2)*(k2[x-1]))*psi[x-1])/(1 + (1/12)*(l**2) * (k2[x+1])).
```

To find, for example, the ground state solution, a trial energy $\epsilon = -0.99$ and constant $\gamma^2 = 200$ were first chosen. Then since $\psi(0) = 0$ such that the boundary condition on the left is satisfied, it will only be satisfied on the right when the trial energy ϵ is the same as an energy eigenvalue of a real physical solution. A tolerance value 10^{-6} was chosen and the trial energy was updated until $\Delta\epsilon < tolerance$ as can be seen in the following snippet.

```
while abs(dE) > tol:
    if (wave(E)[N-1] * wave(E+dE)[N-1] > 0):
        E = E + dE
    elif (wave(E)[N-1] * wave(E+dE)[N-1] < 0):
        dE = dE - dE/2
```

Then to normalise the solutions, the normalisation condition was applied and the solutions were multiplied by a factor of $[\int_0^1 \psi^2]^{-1}$ which was computed using the Simpson's rule integration command in python. To compute the uncertainty in $\tilde{x}$ and $\tilde{p}$ the following formulae were implemented for the uncertainty and expectation values of the

operators

$$\langle \tilde{x}^n \rangle = \int_0^1 \tilde{x}^n \psi(\tilde{x})^2 d\tilde{x}, \qquad \langle \tilde{p}^n \rangle = \frac{1}{i} \int_0^1 \psi(\tilde{x}) \frac{\partial^n \psi}{\partial \tilde{x}^n} d\tilde{x}, \qquad \Delta\xi = \sqrt{\langle \xi^2 \rangle - \langle \xi \rangle^2}. \quad (3.2)$$

In a symmetric potential, $\langle \tilde{x} \rangle$ takes the central value of the potential. Since expectation values only take the real components, we note that since ψ is real and stationary only even powers of momentum have a non-zero expectation value. To compute the second derivative in $\langle \tilde{p}^2 \rangle$ the three point formula was used as shown in the snippet below.

```
sdpsi = np.zeros(N)
    for x in range(1,N-1):
    sdpsi[x] = (norm_psi[x-1] - 2*norm_psi[x] + norm_psi[x+1])/(l**2)
```

4 Results and Discussion

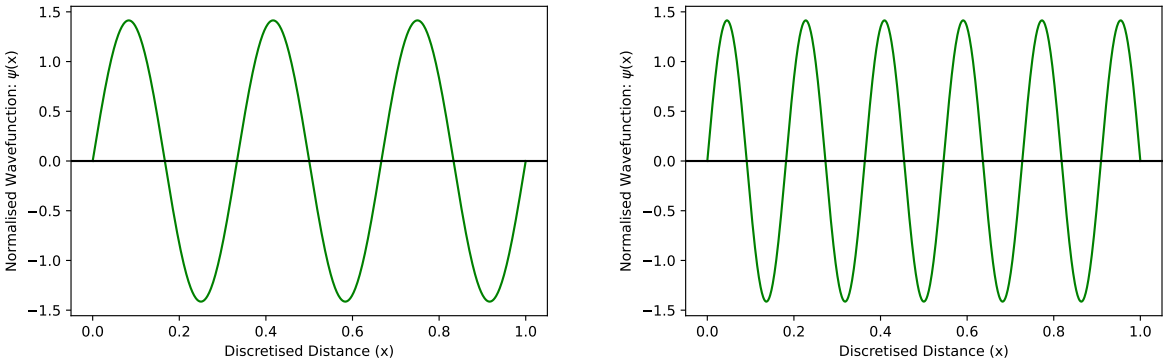
Infinite Square Well Potential
With a chosen tolerance of $tol = 10^{-6}$, the first ten energy eigenvalues were computed using the Numerov method and the results are shown in Table 4.1 below along with the analytical solutions for comparison.

Table 4.1: The first ten energy eigenvalues of the infinite square well potential. $\gamma^2 = 200$

n	Trial Energy (ϵ)	Eigenvalue $\epsilon + \Delta\epsilon = E_n$	Analytical Solution
1	-0.99	-0.9506523	-0.9506520
2	-0.94	-0.8026086	-0.8026079
3	-0.79	-0.5558680	-0.5558678
4	-0.54	-0.2104320	-0.2104317
5	-0.20	0.2337008	0.2337006
6	0.24	0.7765289	0.7765288
7	0.78	1.4180523	1.4180531
8	1.42	2.1582727	2.1582734
9	2.16	2.9971898	2.9971897
10	3.00	3.9348023	3.9348022

The values obtained for an accuracy of 10^{-6} are correct up to this order exactly thus the eigenvalues are as accurate as our chosen tolerance. After changing the tolerance to a smaller value 10^{-8} it was found that indeed the results were even closer to the exact analytical solutions however the computation time required increased significantly.

After applying Simpson's rule to find the appropriate factor, the normalised solutions were plotted and can be seen below in Figure 4.1.



(a) $n = 5$ (b) $n = 10$

Figure 4.1: Plots of the normalised solutions $\psi_n(\tilde{x})$ for the infinite square well potential.

As expected, we see that at the energy eigenvalues ϵ_5 and ϵ_{10}, the wave function satisfies the boundary conditions at $\tilde{x} = \{0, 1\}$. The following values were found for the uncertainty product $\Delta\tilde{x}\Delta\tilde{p}$ for the first ten energy eigenstates.

Table 4.2: Uncertainty products $\Delta\tilde{x}\Delta\tilde{p}$ for the first ten eigenstates of the infinite square well.

Eigenvalue Number (n)	Uncertainty $\Delta\tilde{x}\Delta\tilde{p}$
1	0.56786158
2	1.67028711
3	2.62719481
4	3.55799199
5	4.47898046
6	5.39517902
7	6.30866788
8	7.22046830
9	8.13114086
10	9.04101879

These results show clearly that $\Delta\tilde{x}\Delta\tilde{p} \geq 0.5$ for all energy eigenvalues and therefore the Heisenberg uncertainty relation is obeyed for our system. The uncertainties scale linearly as a function of n and a plot can be found in Figure 6.1.

Harmonic Potential in an Infinite Square Well

With the potential changed to the form shown below in (4.1)

$$\nu(\tilde{x}) = 8(\tilde{x} - 0.5)^2 - 1, \qquad 0 < \tilde{x} < 1, \tag{4.1}$$

we see that now we have a harmonic potential that is also bounded by the infinite square well as in the previous analysis. Plots of the normalised solutions for this potential can

be found in Figure 6.2. Using the Numerov algorithm, the first ten energy eigenvalues were computed and tabulated in Table 4.3, now using a tolerance of 10^{-7} for greater accuracy.

Table 4.3: The first ten energy eigenvalues of the harmonic potential in an infinite well. Note that we have now set $\gamma^2 = 1000$.

n	Trial Energy (ϵ)	Eigenvalue $\epsilon + \Delta\epsilon = E_n$
0	-0.99	-0.9105573
1	-0.91	-0.7316718
2	-0.79	-0.5527862
3	-0.54	-0.3738989
4	-0.20	-0.1949976
5	0.24	-0.0160098
6	0.78	0.1633772
7	1.42	0.3441653
8	2.16	0.5286915
9	3.00	0.7208755

From this table, we notice that the distance between adjacent energy levels is constant for lower energy states but then begins to vary as n increases, to investigate this behaviour the next ten energies were calculated and the adjacent distance was plotted as a function of n which can be seen in Figure 4.2.

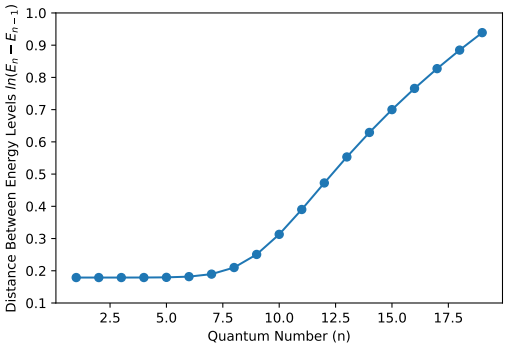


Figure 4.2: The logarithmic distance between the first 20 energy levels in the harmonic potential with infinite well boundaries as a function of the quantum number n

The sharp increase in adjacent energy level distance can be explained by considering the potential as being a combination of the infinite square well and harmonic potentials. Since these two potentials are separable mathematically, the energy solutions will have components of the form $\omega(n + \frac{1}{2})$ and $\pi^2(n)^2/\gamma^2$. The harmonic component is linear in n while the boundary component is quadratic in n. So for small n the linear term will

dominate leading to approximately the same solutions as the harmonic oscillator, and as n grows larger the quadratic term takes over causing the distance to scale non-linearly.

Repeating the same calculations of $\Delta\tilde{x}\Delta\tilde{p}$ for the second case, results were obtained as seen in Table 4.4.

Table 4.4: Uncertainty products $\Delta\tilde{x}\Delta\tilde{p}$ for the first ten eigenstates of the harmonic potential within an infinite square well.

Eigenvalue Number (n)	Uncertainty $\Delta\tilde{x}\Delta\tilde{p}$
0	0.499998
1	1.499986
2	2.499964
3	3.499941
4	4.499985
5	5.500491
6	6.503049
7	7.511683
8	8.530690
9	9.554935

From this table, we see that the uncertainty of each state approximately obeys $(\Delta\tilde{x}\Delta\tilde{p})_n = (\Delta\tilde{x}\Delta\tilde{p})_{n-1} + 1$. In addition to this we also see that the ground state ($n = 0$) is a minimum uncertainty state. This implies that its wavefunction is a Gaussian wavepacket.

5 Conclusions

In this experiment I showed that the accuracy of energy eigenvalues for a given potential found by the Numerov algorithm are directly dependent on the choice of tolerance. The tolerance is how close we allow the adjustment $\Delta\epsilon$ to come to zero before truncating the algorithm for our final result. As we saw, lowering the tolerance can rapidly increase the computation time required for the algorithm. The eigenstates $\psi_n(\tilde{x})$ which necessarily satisfied the boundary conditions of each problem (as solutions of the Numerov method) were able to be plotted and successfully represented the distribution of the probability.

The energy eigenvalues and uncertainties computed using a discrete distribution of points in $\tilde{x}$-space were in agreement with the theory discussed on these potentials verifying the integrity of the approximation methods used in python such as Simpson's rule and the three point formula for integration and differentiation.

In the particularly interesting case of the harmonic potential bounded by a square infinite well, the distance between adjacent energy levels displayed a strange behaviour in that it was constant for small n and began to increase for larger n. This result was explained by the respective linear and quadratic dependence on the quantum number in each separated component of the potential.

6 Appendix

6.1 References

[1]: Laboratory Handout "Numerical solution of the time-independent 1-D Schrodinger equation" - Paul Eastham, Mark Mitchison, Matthias E. Mobius School of Physics Trinity College Dublin.

6.2 Additional figures

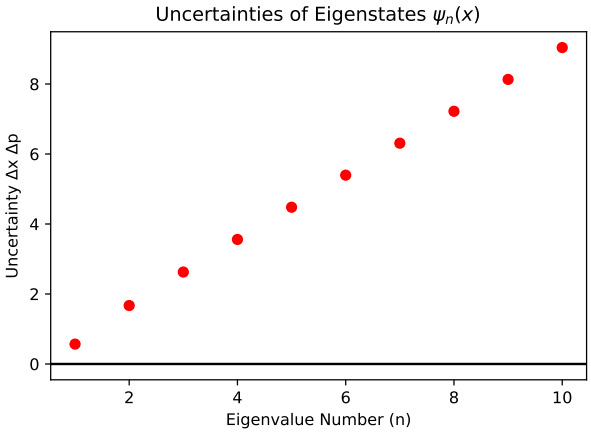
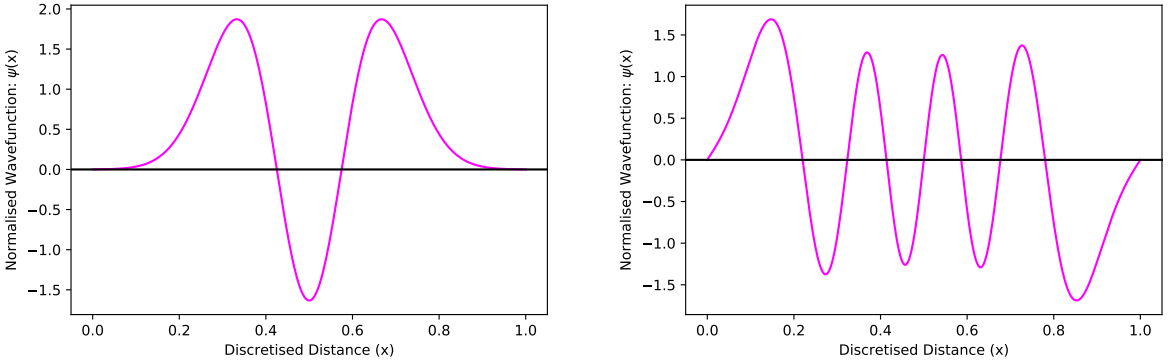


Figure 6.1: A plot of the uncertainties $(\Delta\tilde{x}\Delta\tilde{p})_n$, obtained for the infinite square well potential.



(a) $n = 3$ (b) $n = 8$

Figure 6.2: Plots of some normalised solutions $\psi_n(\tilde{x})$ for the harmonic potential within an infinite square well.