

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

Gavin Cheung



09328173

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Abstract

The 1-D time independent Schrodinger Equation is solved numerically using the Numerov algorithm. We first took the potential in an infinite square well. This has an analytic solution and we compared the numerical results. It was found that the numerical and analytical solutions agreed with each other. We then look at the step potential and the linear potential and find numerical solutions. We also check orthogonality for the different eigenfunctions which is confirmed.

★ Introduction

The time-independent 1-D Schrodinger Equation is

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

where $\psi(x)$ is the wavefunction, $V(x)$ is the potential and m is the mass. In general, it is not easy to find an analytic solution so we must resort to numerical methods.

1) However, for a particle in a box,

$$V(x) = \begin{cases} V_0 & \text{if } |x| < L \\ \infty & \text{if } |x| \geq L \end{cases}$$

then it is possible to find an analytic solution. Take ansatz $\psi = A \sin cx + B \cos cx$. The boundary conditions are $\psi(0) = 0$ and $\psi(L) = 0$. This gives $c = \frac{n\pi}{L}$ and $B = 0$. Finally, requiring the normalising condition, $\int_{-\infty}^{\infty} \psi^2 dx = 1$ gives $A = \sqrt{\frac{2}{L}}$. Thus, our analytic solution is $\psi(x) = \sqrt{\frac{2}{L}} \sin \frac{n\pi}{L} x$. Finally, substituting this back into the Schrodinger Equation gives the energy values,

$$E_n = \left(\frac{\hbar^2 n^2 \pi^2}{2mL^2} - V_0 \right)$$

In computation, it is often convenient to nondimensionalise x . The nondimensionalised Schrodinger Equation is

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

where $\nu(\tilde{x}) = \frac{V(\tilde{x})}{V_0}$, $\epsilon = \frac{E}{V_0}$ and $\gamma^2 = \frac{2mL^2 V_0}{\hbar^2}$. This equation would give energy values

$$\epsilon_n = \frac{\pi^2 n^2}{\gamma^2} - 1$$

For some more complicated potentials, we can only work numerically. Our goals will be to compare the analytic and numerical solution of the constant potential. Then we will numerically solve the Schrodinger equation for a step and linear potential. We will also check orthogonality of different eigenfunctions. This is a simple result from linear algebra if our observables are Hermitian.

★ Experimental Method

The Numerov algorithm will be employed to integrate the equation. We will start with the boundary conditions $\psi(x_0 = 0) = \psi(x_{N-1} = 1) = 0$. The next points $\psi_{left}(x_1)$ and $\psi_{right}(x_{N-2})$ are arbitrary. We will then find the points $\psi_{left}(x_2)$ and $\psi_{right}(x_{N-3})$ using the Numerov algorithm. This process is repeated until we get to the matchpoint as we shoot from the left and right. We will take the total number of points $N = 1000$. Thus our step size is $l = 1/(N - 1)$. Also, we take $Matchpoint = N/2$, and $\gamma^2 = 100$.

2) A template is used. The program is compiled and plots are made for a number of trial energies.

3) If the trial energy is not a solution, the slope will be discontinuous at the matchpoint. The code is modified so that it computes the differences in slopes of ψ_{left} and ψ_{right} . The difference in slopes is verified manually to be a minimum at an eigenstate.

4) The code is modified so that starting with some trial energy E , the energy is continuously incremented by some value ΔE until the difference in slopes changes sign. Then set $\Delta E = -\Delta E/2$ and repeat. Terminate this procedure once a suitably small value of ΔE has been reached.

5) Compare the ground state energy found numerically with the analytical solution.

6) Even eigenvalues ($\epsilon_2, \epsilon_4, \dots$) cannot be found from this method. The reason why is because even eigenvalues have odd eigenfunctions. Near one of the boundaries, the function is negative but the program will always start with a positive initial point. Modify the code by setting the initial point $\psi_{right} = -0.0001$. However, the program is now unable to find odd eigenvalues.

7) In order to be able to find both even and odd eigenstates, we choose a different matchpoint that is not in the middle. ψ_{right} is then rescaled by a factor $\frac{\psi_{left}(matchpoint)}{\psi_{right}(matchpoint)}$. This does not affect the solution since if ψ is a solution to the S-eqn, then $c\psi$ is also a solution. Note that problems may occur if the function is zero at the matchpoint and we multiply/divide by zero.

8) Using the modified code, find the first six energy eigenstates and verify that they agree with the analytical solution.

9) Normalise the eigenfunctions. Use Simpson's rule to numerically integrate $\int_0^L \psi(x)^2 dx$. Then divide the eigenfunction by the integral.

10) Change the potential to that of a step potential where $\nu(x) = -1$ for $0 < x < 0.5$ and $\nu(x) = 0$ for $0.5 < x < 1$.

11) Find the first six energy eigenstates of this potential. Then find the probability for the particle to be in the right half of the well by calculating $\int_{0.5}^L \psi(x)^2 dx$ using Simpson's Rule.

12) Verify that the eigenfunctions are orthogonal by using Simpson's rule to integrate $\int_0^L \psi_1 \psi_2 dx$ where ψ_1 and ψ_2 are distinct eigenfunctions.

13) Change the potential to that of a linear potential and find the first six energy eigenstates.

★ Results and Analysis

2) Our first energy state is $\frac{\pi^2}{100} - 1 \approx -0.901$. Figure 1a shows the wavefunction for energy value -0.901 . The slope appears continuous at all points so this is approximately a solution. Taking $E = -2$ and $E = 1$ gives drastic discontinuities in slope so these cannot be solutions.

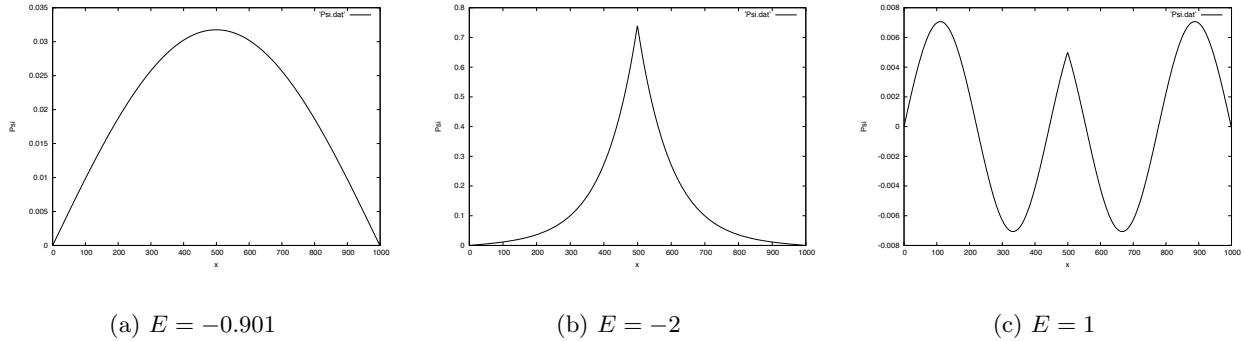


Figure 1: Wavefunctions for several Trial Energies

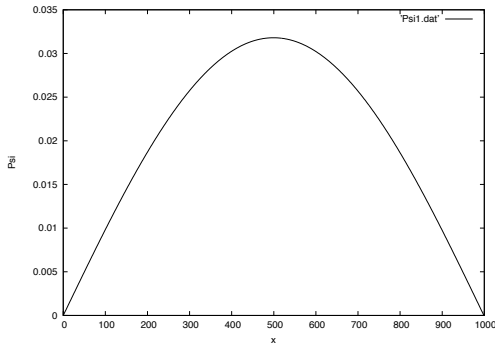
3) For $E = -0.901$, the difference in slopes is 0.000000. For $E = -2$, the difference is 0.014842. For $E = -0.8$, the difference is -0.000123 . It is clear from this that the slope difference is minimised at the energy eigenstate.

5) The first energy eigenstate of the constant potential is found to be -0.901303955991 . Compared with the analytical solution $\frac{\pi^2}{100} - 1$ which is given as ≈ -0.901303955989 using Wolfram, this is a very good approximation. We can always make our solution more accurate by decreasing the cutoff point of ΔE .

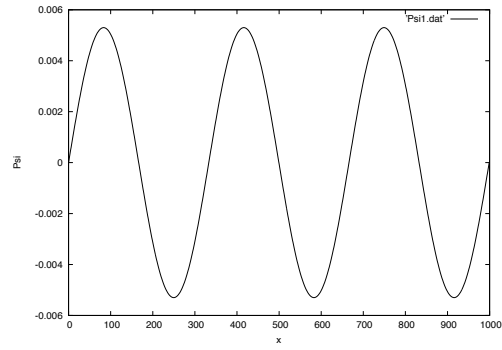
8) The first six energy eigenstates are found to be

Numerical Energy Eigenstates
1) -0.901303955991
2) -0.605215823960
3) -0.111735603929
4) 0.579136704010
5) 1.467401099644
6) 2.553057582514

which correspond to the analytical values. Figure 2 shows some examples of the eigenfunctions.



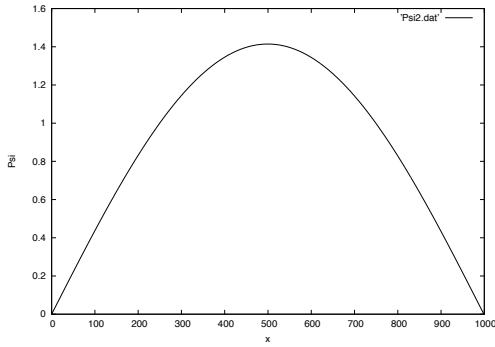
(a) $E \approx -0.901$



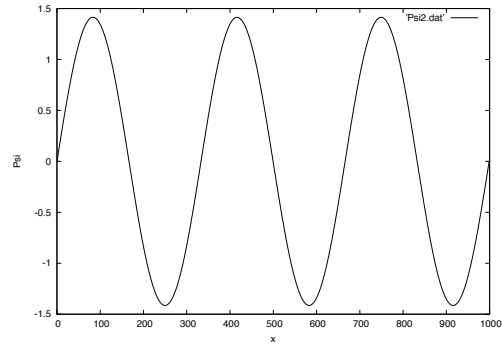
(b) $E \approx 2.5$

Figure 2: Non-normalised Wavefunctions for Constant Potential

9) Figure 3 shows the normalised eigenfunctions. Note that they have the same shape as the non-normalised eigenfunctions. The only difference is the multiplicative factor to ensure $\int_0^L \psi(x)^2 dx = 1$.



(a) $E \approx -0.901$



(b) $E \approx 2.5$

Figure 3: Normalised Wavefunctions for Constant Potential

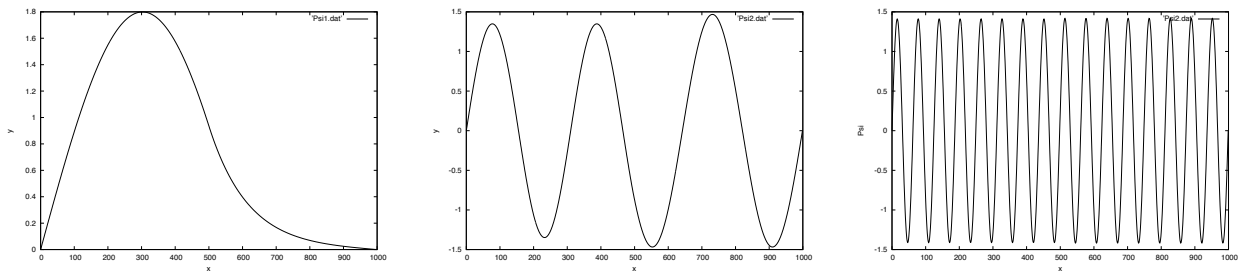
11) The first six energy eigenstates for the step potential are

Numerical Energy Eigenstates	
1)	-0.731329364535
2)	-0.023988677211
3)	0.436729627010
4)	1.152688182963
5)	1.959921830059
6)	3.095349541988

The probabilities for the particle to be in the right hand side for various energy eigenstates are given here

Energy(approx)	Probability
-0.7	0.052885
0.5	0.739494
5	0.546858
10	0.523734
50	0.500862
100	0.503602
1000	0.502769
10000	0.500444

It can be seen that the probability approaches 0.5 for large values of energy. This can be explained easily. As the energy increases, the step potential becomes negligible since the difference is only 1. We can then neglect the step and treat it as a constant potential which would have right hand side probability 0.5. This is apparent in figure 4c.



(a) $E \approx -0.7$

(b) $E \approx 3$

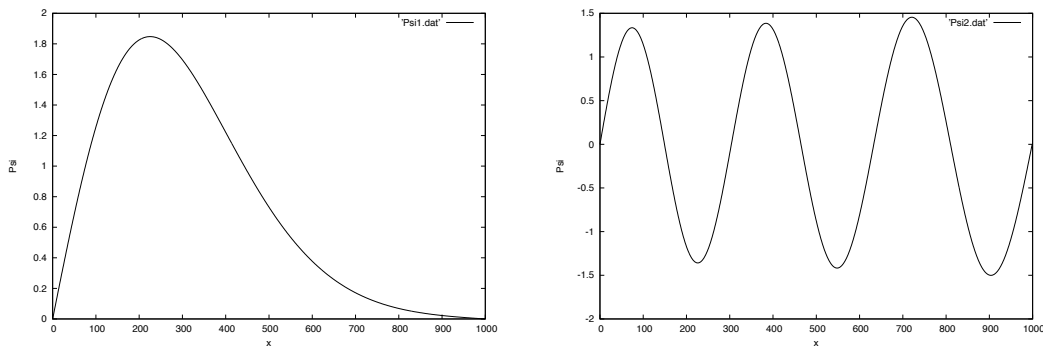
(c) $E \approx 100$

Figure 4: Normalised Wavefunctions for Step Potential

12) As expected, we have verified that the eigenfunctions are orthogonal.

13) The first six energy eigenstates of the linear potential are given,

Numerical Energy Eigenstates	
1)	-0.200361833826
2)	0.401537681602
3)	0.951206587193
4)	1.626016836598
5)	2.499172564993
6)	3.575583994743



(a) $E \approx -0.2$

(b) $E \approx 3.5$

Figure 5: Normalised Wavefunctions for Linear Potential

★ Conclusion

We have verified that the Numerov algorithm is sufficient in finding the solutions to the constant potential when comparing with the analytical solution. Thus, we were then able to find the solutions to the step potential and linear potential. Looking at the step potential, we found that for high energies, the probability for the particle to be in the right hand side of the well tends to 0.5 which can be reasoned by assuming the step is negligible. Another major result is that the eigenfunctions are orthogonalised which is a result from Quantum Mechanics.