

Computation Lab - Nonlinear Pendulum

Chris Kervick - 11355511

November, 2013

Abstract

A computer program was utilised to numerically calculate solutions to the time-independent, 1-D Schrödinger equation. In the case of an infinite square well potential, these numerical solutions were found to match the analytic solutions. Solutions were then calculated for the cases of step and linear potentials. The eigenfunctions calculated were found to be orthogonal.

Aims

- To calculate the first 6 energy Eigenstates for an infinite square well potential, a step potential and a linear potential.
- To normalise the corresponding Eigenfunctions.
- To check the orthogonality of these Eigenfunctions.

Introduction and Theory

The general form of the time-independent, 1-D Schrödinger equation is

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

with $\psi(x)$ the wavefunction, E the particle's energy, m the particle's mass and $V(x)$ the potential function.

In the case of a so-called *particle in a box*, this equation can be solved analytically. We have

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

and we make the ansatz $\psi(x) = A\sin(cx) + B\cos(cx)$. The boundary conditions $\psi(0) = \psi(L) = 0$ imply $B = 0$ and $c = \frac{n\pi}{L}$. To find the remaining constant, A , we impose that the probability be normalised, i.e. $\int_{-\infty}^{\infty} |\psi(x)|^2 dx = 1$, which gives $A = \sqrt{\frac{2}{L}}$. Substituting these constants back into the original equation gives $\psi(x) = \sqrt{\frac{2}{L}}\sin(\frac{n\pi}{L}x)$. Substituting this expression for ψ back into the original Schrödinger equation gives the energy levels,

$$E_n = \frac{h^2 n^2}{8mL^2} - V_0$$

For computational purposes, we nondimensionalise the Schrödinger equation as follows:

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

where $\gamma^2 = \frac{2mL^2V_0}{h^2}$, $\epsilon = \frac{E}{V_0}$ and $\nu = \frac{V(\tilde{x})}{V_0}$

In other cases (e.g step potential, linear potential), we must work numerically. In this experiment we will compare the analytic and numerical solutions to the infinite square well potential, and then numerically solve the cases of step and linear potentials. We can also numerically normalise the eigenfunctions and check their orthogonality.

Experimental Method

The wavefunctions and energy eigenstates were calculated numerically using the Numerov Algorithm. To do this, the following details were used: the interval $[0, 1]$ was divided into N points, with N being set to 1000; the potential was initialised as an infinite square well potential; the boundary conditions $\psi(x_0) = \psi(0) = 0$ and $\psi(x_{N-1}) = \psi(1) = 0$ were set, with $\psi(x_1)$ and $\psi(x_{N-2})$ being arbitrarily set to 0.0001; the match-point for the Numerov Algorithm was initially set to $\frac{N}{2}$, though this was changed in certain cases; γ^2 was set to 100.

Through trial and error, it was noted that the analytically calculated energy eigenstates occurred when the slope difference at the match-point was minimised; that is to say when the slopes found by shooting from the left and shooting from the right were continuous at the match-point. Thus, the program was edited to find such points. Departing slightly from the recommended method, it was instead decided to achieve this as follows:

The slope difference at the match-point was calculated via the Euler difference method ($\psi'(x) \approx \frac{\psi(x+l)-\psi(x)}{l}$). This slope difference was calculated for $-2 \leq E \leq 5$ for increments of E of 0.00001, leading to a data set of slope difference at match-point versus E . The points where this slope difference reached zero were then printed, leading to a list of all energy eigenstates in the range. By scaling ψ_{right} by $\frac{\psi_{left}(Match-point)}{\psi_{right}(Match-point)}$ (allowed since solutions to the Schrödinger equation can always be multiplied by an arbitrary constant) and by choosing a suitable match-point, this method printed both even and odd eigenstates.

The corresponding Eigenfunctions were then normalised. This was achieved by using Simpson's rule for numerical integration to calculate

$$\int_{x_0=0}^{x_{N-1}=1} \psi(x) dx.$$

To normalise, ψ was then multiplied by the inverse of this numerical result.

The form of the potential was then changed to a step potential, and the eigenstates found by the same method as above. In this case the match-point had to be selected to be outside the bump, to avoid integrating into a classically forbidden region where ψ would be complex. Again using Simpson's method, the probability was calculated for the particle to be located in the right half of the well, and the asymptotic value of this probability was found for E approaching ∞ . The orthogonality of these eigenfunctions was checked by using Simpson's rule to integrate them against one another.

Finally, the form of the potential was changed to that of a linear potential, and the eigenstates again found by the slope-difference method.

Results and Analysis

Using the modified Eigenstate program, the following energy eigenstates were found as the first 6 Eigenstates for the infinite square potential.

No.	Energy Eigenstates
1	-0.90093
2	-0.6030
3	-0.11101
4	0.58167
5	1.48209
6	2.56322

Table 1: Energy Eigenstates of Infinite Square Potential

It was verified that the slope difference was indeed minimised at each of the eigenstates. ψ was plotted at these points to ensure their validity. An example of such a plot can be found below, with further examples in the appendix.

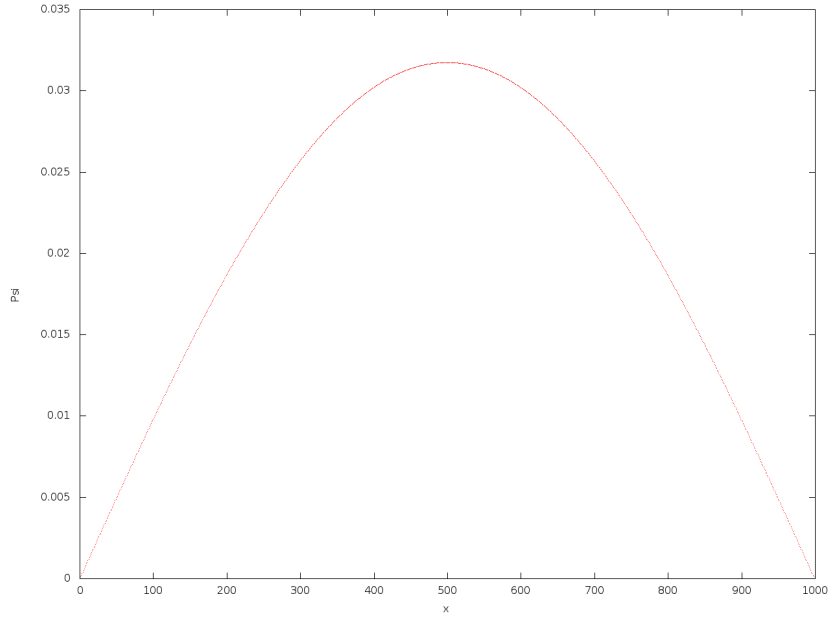


fig 1: ψ plotted for $E = -0.90093$

The normalisation constant was calculated numerically. Below is a plot of the same Eigenstate as is plotted above but in this case normalised.

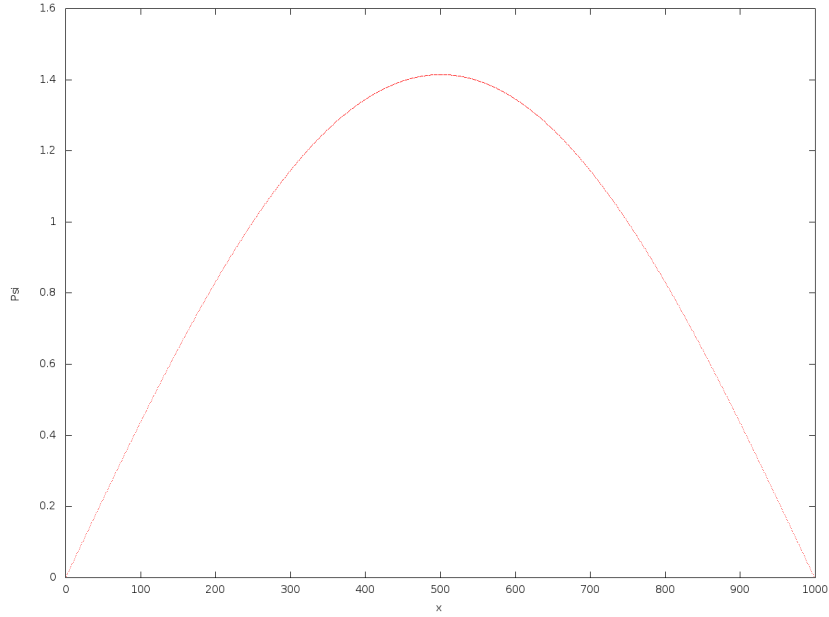


fig 2: Normalised ψ plotted for $E = -0.90093$

As we can see, the only difference is the y-axis scaling result from multiplication by the normalisation constant

Below is a table of the first 6 energy eigenstates of the step potential.

No.	Energy Eigenstates
1	-0.72871
2	-0.02357
3	0.43730
4	1.16228
5	1.97447
6	3.09797

Table 2: Energy Eigenstates of Step Potential

It was seen clearly that the probability for the particle to be in the right half of the well asymptotically approached 0.5 for large energies. This corresponds to the fact that a potential step of 1 can be seen as negligible for particles with sufficiently high energies. It was also noted that while the probability was rather small in the case where the particle had an energy smaller

than that of the step, it was in fact non-zero indicating a small degree of tunnelling. This is shown in the appendix by two plots of the probability $|\psi|^2$ (figs A4, A5).

It was found that indeed these eigenfunctions were orthogonal to one another, as predicted.

Below is a table of the first 6 energy Eigenstates of the linear potential.

No.	Energy Eigenstates
1	-0.20055
2	0.40449
3	0.95534
4	1.62607
5	2.51269
6	3.58431

Table 3: Energy Eigenstates of the Linear Potential

Discussion and Conclusions

The Numerov Algorithm proved sufficient for calculating the energy eigenstates of the infinite well potential, as compared with the analytically achieved results. Thus one can have confidence in the results obtained for the step and linear potentials. Also of note the fact that the probability for the particle to be in the right half of the well approached 0.5 for high energies. This corresponds with the fact that the step becomes negligible for sufficiently high energy. Further adding to the confidence in our results is the fact that the eigenfunctions were orthogonal, a well-known result from quantum mechanics.

Appendix of diagrams

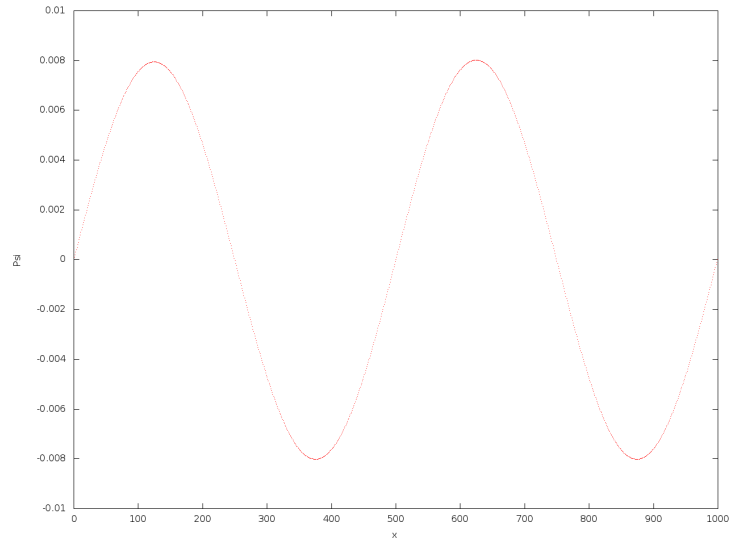


fig A1: Fourth energy state of infinite well potential, $E = 0.58167$

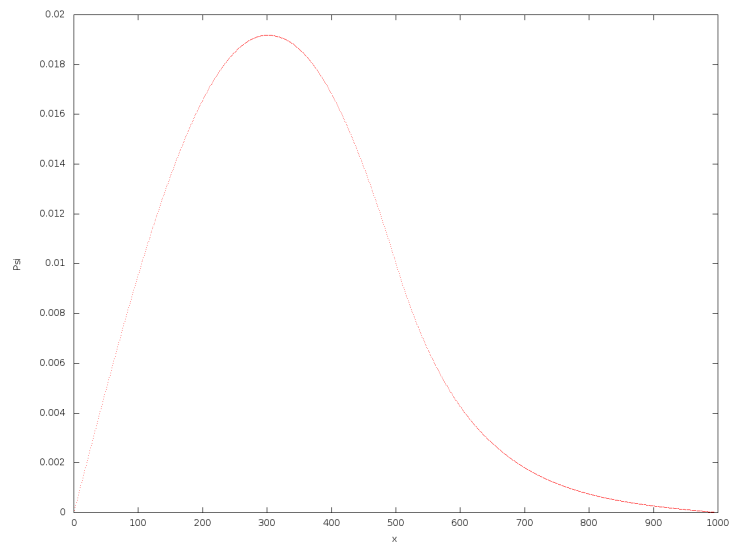


fig A2: Wavefunction for step potential, $E = -0.72871$

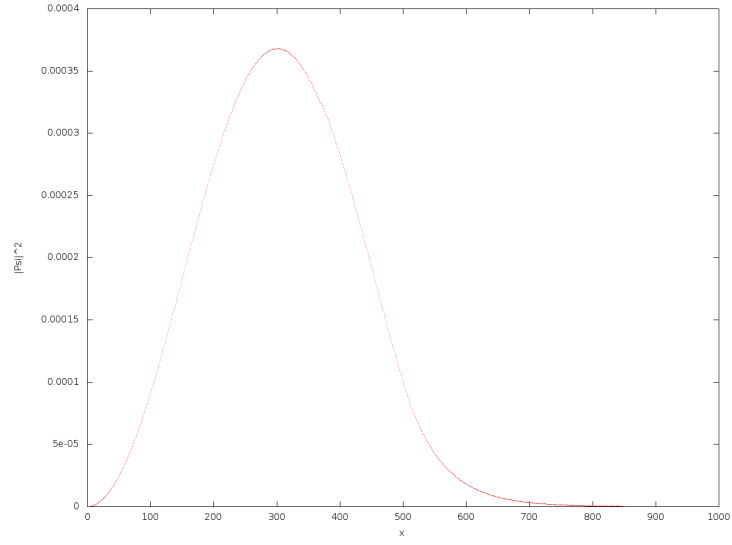


fig A3: Probability distribution of above wavefunction, $E = -0.72871$

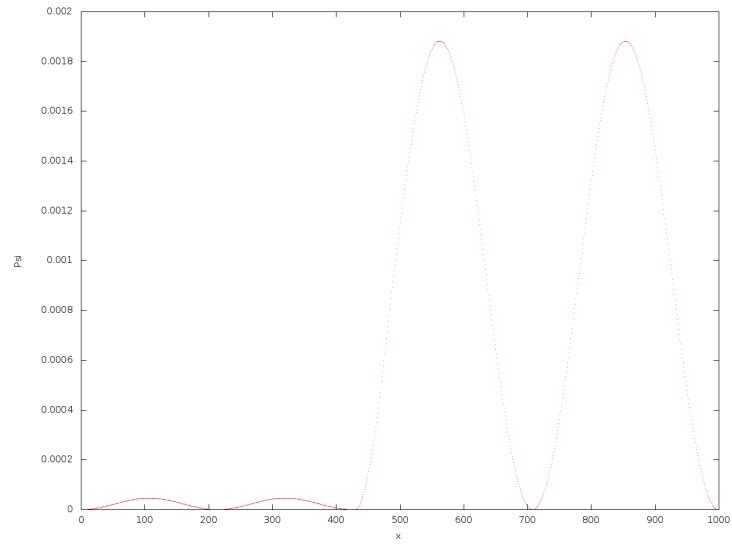


fig A4: Probability distribution for step potential, $E = 1.97447$. Notice the negligibility of the step.

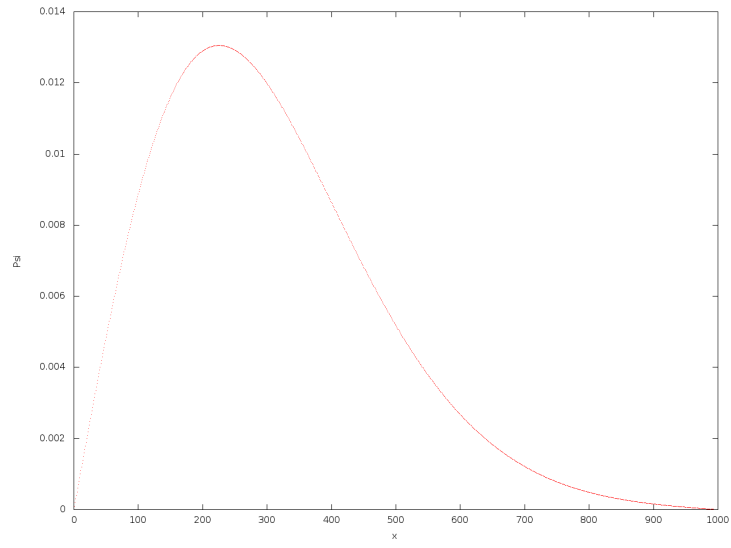


fig A5: Wavefunction for linear potential, $E = -0.20055$

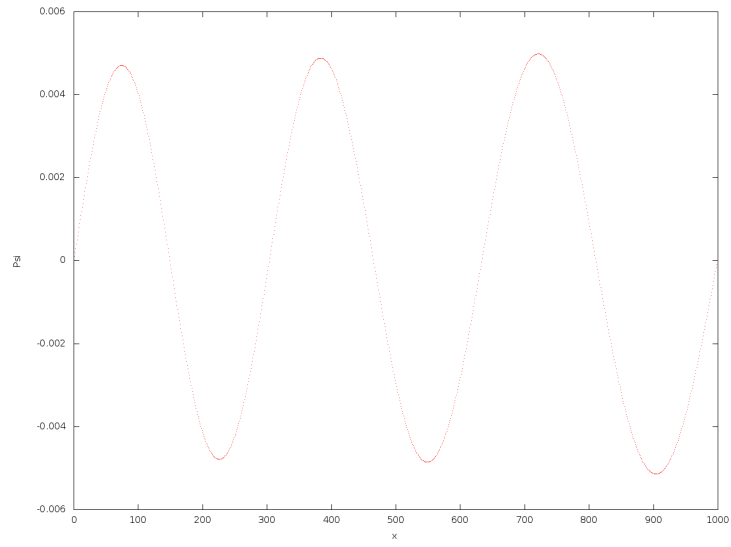


fig A6: Wavefunction for linear potential, $E = 3.58431$