EXP – 6

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Aim: Using the Numerov method to solve the Schrodinger's equation for a particle in a box, and find the energy eigen values and the wavefunctions for the ground and the first 3 excited states.

Theory:

For a particle in 1D box, we know,

$$\psi(x) = A \sin\left(\frac{n\pi x}{L}\right)$$

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

In its lowest energy state, particle in a box is mostly likely to be in the middle of the box.

But for next energy state, $|psi|^2 = 0$ at x = 0.5L

We implement the Numerov algorithm to solve the Schrodinger's equation for particle in box.

The Schrödinger equation is a second order differential equation used in quantum mechanics to determine the wavefunctions and eigenstates of a system. It is typically of the form

$$\left(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)\right)\Psi_n(x) = E_n \Psi_n(x), \quad \text{------ (1)}$$

here Ψ (x) are the wavefunctions, En are the eigenstates and V (x) is some potential. For simplicity, they shall be used in this experiment, as the known analytic solutions can provide useful insight to the validity of the numerical solutions where Ψn (x) are the wavefunctions, En are the eigenstates and V (x) is some potential.

For simplicity, the particle will be contained in an infinite well, obtained by the boundary conditions: V (0) = V (L) = ∞, where L is the length of the well. It is difficult to solve (1) for an arbitrary potential.

The most well-known analytic solutions to (1) are in the cases of the square well and harmonic potentials. They shall be used in this experiment, as the known analytic solutions can provide useful insight to the validity of the numerical solutions.

It is convenient to work with a dimensionless form of (1) in order to avoid working with factors of ~. It can be re-written as

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

Since (2) is of the form

$$\frac{d^2}{dx^2}\Psi(x) + k^2(x)\Psi(x) = 0, \qquad (3)$$

where $k^2(x) = \gamma^2(\epsilon - \nu(\tilde{x}))$ in this case, it can be integrated using the Numerov algorithm. By defining ~x with a discrete set of N points, separated by a distance l = 1/(N−1), (2) can be written in discrete form:

$$\frac{d^2}{d\tilde{x}^2}\Psi_n + k_n^2\Psi_n = 0,$$

The integration scheme is given by

$$\Psi_{n+1} = \frac{2\left(1 - \frac{5}{12}l^2k_n^2\right)\Psi_n - \left(1 + \frac{1}{12}l^2k_{n-1}^2\right)\Psi_{n-1}}{1 + \frac{1}{12}l^2k_{n+1}^2}.$$

This algorithm is obtained using Taylor expansions and the central difference method. While it could be solved using Runge-Kutta, this method takes advantage of the fact that (2) is linear in Ψ and contains only its second derivative.

ALGORITHM:

- Mesh parameters: h and x_m.
- Accuracy δ for matching logarithmic derivatives
- State specification N, i.e., ground state or higher (N = 1, 2, …).
Note this sets the parity in the present case. The number of nodes is: N – 1.
We set N = 1.
- Trial energy ε_t and matching point x_c = 0.

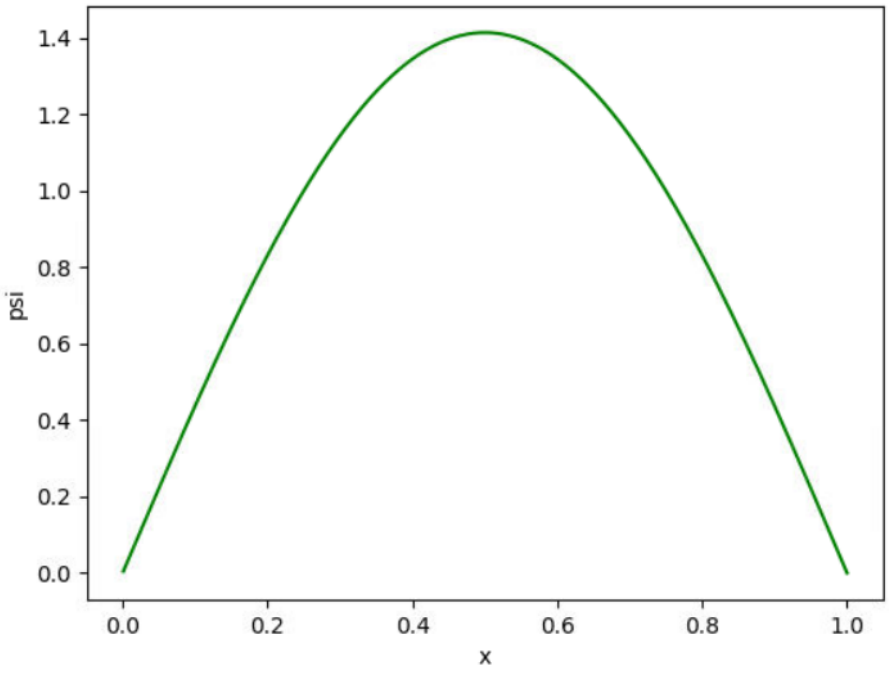
• Begin iteration for finding eigenvalue
- Set $\varepsilon_l = \varepsilon_t$.
- Initialize y_1 and y_2 as y_1 = 0 and $y_2 = a$ small constant.
- Use forward relation to obtain solution till x_c.
- Calculate γ_l.
- Initialize y_n and y_{n-1} as y_n = 0 and y_{n-1} = a
small constant. Note: $x_n = x_m$, the rightmost point on the mesh.
- Use backward relation and obtain γ_r at x_c.
- Calculate $err = \gamma_l - \gamma_r$.
- Increase trial energy until *err* changes sign. Denote this energy as ε_u. The eigenvalue is now bounded between ε_l and ε_u.
- Use a suitable root finding algorithm, e.g., bisection method, to find the energy ε_b so $|err| \leq$ δ, the desired accuracy.
- Match the values of left and right wave function at x_c and use the scale one of the wave functions to obtain a continuous Eigen Function.
- Normalize the entire wave function.

Observations:

We write the code for calculating the energy Eigen values for the ground and the first 3 excited states.

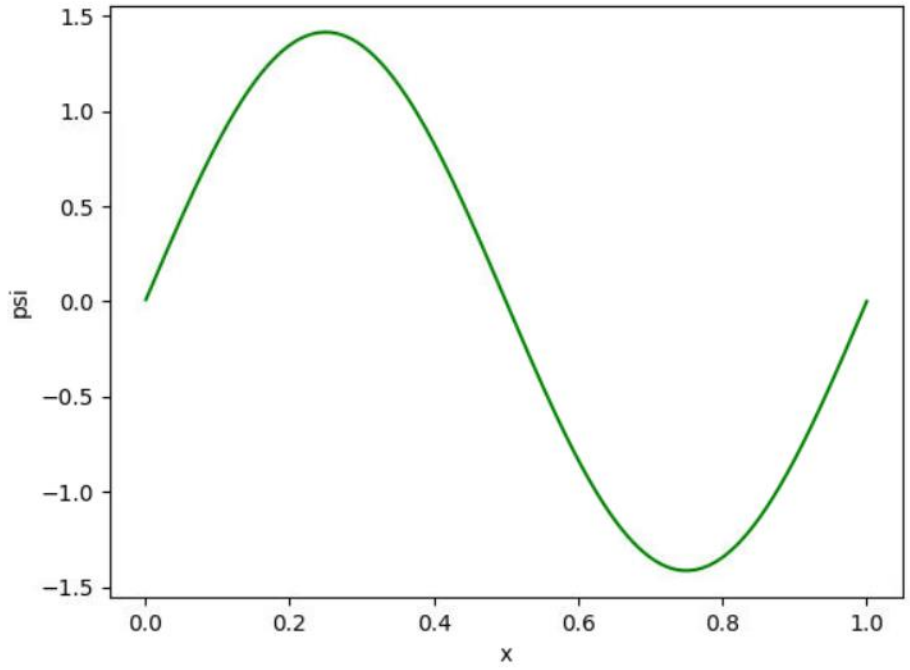
Here are the plots of the wave functions for the ground state and the first 3 excited states:

For ground state (n = 1),



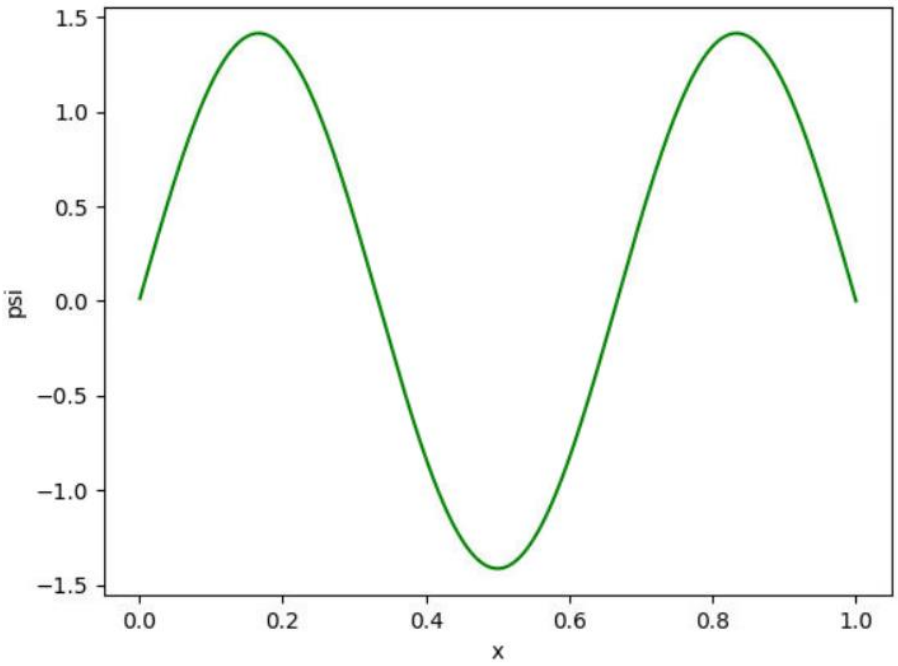
We get energy E as 6.056263736263735e-38.

For 1st excited state (n = 2):



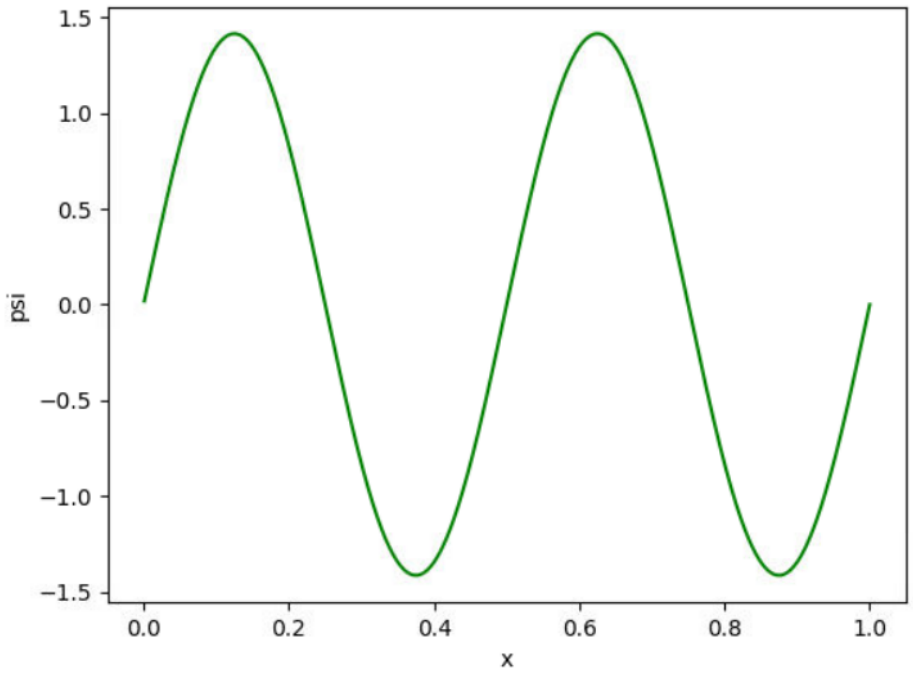
We get energy E as 2.422505494505494e-37.

For 2nd excited state (n = 3):



We get energy E as 5.450637362637362e-37.

For 3rd excited state (n = 4):



We get energy E as 9.690021978021976e-37.

Code:

The code for the plots shown above has been attached with this report, and can be run using **python Exp6.py**