Numerical solution for 1-D infinite potential problem.

Assignment #2

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For the students who are studying the quantum mechanics, the 1-D infinite potential problem is very basic problem to understand the wave property.

In this assignment, we use infinite potential problem using numerical method.

The Schrodinger equation is as follows:

$$\frac{\hbar^2}{2\mathrm{m}}\nabla^2\Psi + \mathrm{V}\Psi = \mathrm{E}\Psi$$

Where m is the mass of the particle, $\hbar$ is the Planck constant ($\frac{\mathrm{h}}{2\pi}$), V is the scalar potential, and E is the energy of this system. (a is the width of the well)

When we solve the Schrodinger equation we can get the wave equation and energy eigenvalue. The analytical solution for 1-D infinite potential well problem is as follows:

$$\frac{\hbar^2}{2\mathrm{m}}\nabla^2\Psi = \mathrm{E}\Psi$$

Using the Boundary condition ($\Psi(0) = \Psi(\mathrm{a}) = 0$), we can let the $\Psi = \sin(\mathrm{kx})$ and $\mathrm{ka} = \mathrm{n}\pi$ then,

$$\nabla^2\Psi = \mathrm{k}^2\Psi \text{ where } \mathrm{k}^2 = \frac{2mE}{\hbar^2}$$

$$\text{otherwise: } \Psi = 0$$

If we let the a=5nm and m=0.19 m_e, we can easily get the energy eigenvalue for the ground state.

E=0.0793 eV

However, for the numerical solution, we cannot calculate the exact solution. So we choose the N points of wavefunction. The larger N gives us the closer eigenvalue. The second derivative of the function can be expressed as:

$$\frac{d^2}{dx^2}\Psi(x_n) \approx \frac{\Psi(x_{n-1}) - 2\Psi(x_n) + \Psi(x_{n+1})}{\Delta x^2}$$

$$\text{Where } \Delta x = \frac{\mathrm{a}}{\mathrm{N}-1}$$

The numerical solution is given in Table 1.

N	Energy (eV)	Error (%)
5	0.0753	5.04
50	0.0792	0.126
500	0.0793	0

The results show there is some error between analytical solution and numerical solution. However, for N = 500 case, the numerical solution and analytical solution is same in three significant figures.