one-particle-in-a-bok

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1 One particle in a box

1.1 Setting model system

Solving the time-independent Schrodinger equation, $\hat{H}\Psi = E\Psi$, for one particle in a box (i.e., finding the wavefunctions and their corresponding energies with given boundary conditions). The Hamiltonian and the boundary condition for the potential are

$$\hat{H} = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x), \text{ and } V = \begin{cases} 0 & \text{if } 0 < x < L \\ \infty & \text{if } x \leq 0 \text{ or } x \geq L \end{cases}$$

where $\hbar$, m are the reduced Planck constant and the mass of particle. This particle is confined in an one-dimensional box with the length from 0 to L that the The postulate wavefunction is

$$\Psi(x) = A\sin(kx) + B\cos(kx),$$

where A and B are unknown coefficients, and k is also unknown.

1.1.1 Tasks

1. Finding the analytical expression for both wavefunction and energy, Ψ and E.
2. If we don't know the analytical solution, how to solve this problem numerically.

1.1.2 Tips

Compare the plots of above analytical and numerical solution.

1.2 Task 1, Analytical solution

Plug postulate wavefunction into Schrodinger equation, $\hat{H}\Psi = E\Psi$. The left hand side is

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} \cdot (A\sin(kx) + B\cos(kx)) = -\frac{\hbar^2}{2m} \cdot (-Ak^2\sin(x) + Bk^2\cos(x)),$$

and then from the boundary conditions, x=0,

$$-\frac{\hbar^2}{2m}(-Bk^2) = 0 \rightarrow B = 0 \rightarrow \Psi(x) = A\sin(kx).$$

The other boundary condition, x=L,

$$-\frac{\hbar^2}{2m}Ak^2\sin(kL) = EA\sin(kL) \rightarrow kL = \pi, 2\pi.... \rightarrow k = \frac{n\pi}{L}, n = 1, 2, 3, ...$$

The energy is

$$E = \frac{\hbar^2}{2m}k^2 = \frac{n^2h^2}{8mL^2}$$

To find the unknown coefficient, consider the normalization condition.

$$\int_0^L |\Psi|^2 dx = 1 \rightarrow \int_0^L \Big[A\sin\big(\frac{n\pi}{L}x\big)\Big]^2 dx = \int_0^L A^2\frac{1}{2}\Big(1-\cos\big(\frac{2n\pi}{L}x\big)\Big)^2 dx = \frac{A^2}{2}L^2 = 1 \rightarrow A = \sqrt{\frac{2}{L}}$$

The wavefunction is $\Psi = \sqrt{\frac{2}{L}}\sin(\frac{n\pi}{L}x)$