PH4074: Computational Physics Lab

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1. **Finite square well potential problem.** Consider the Schrödinger's equation (SE)

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

where $V(x)$ is given by the finite square well potential as shown in Fig. 1.

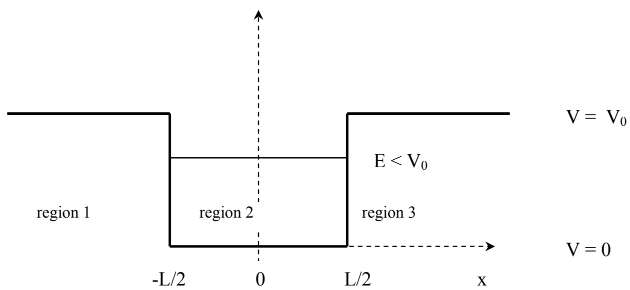

Figure 1: A finite square well, depth, V_0, width L.

To make things easier for computer work let us pick a set of dimensionless variables. Let

$$X \equiv \frac{x}{L}$$

Then the SE can be written as

$$-\frac{d^2\psi(X)}{dX^2} + \frac{2mL^2}{\hbar^2}V(X)\psi(X) = \frac{2mL^2}{\hbar^2}E\psi(X)$$

This suggests defining new dimensionless variables for the energies E and U in terms of the energy $\frac{h^2}{8mL^2}$: $E' = E\frac{8mL^2}{h^2}$ and $V' = V\frac{8mL^2}{h^2}$. Incorporating these, the SE becomes

$$-\frac{d^2\psi(X)}{dX^2} + \pi^2 V'(X)\psi(X) = \pi^2 E'\psi(X)$$

Now let us choose an equally spaced set of value of x given $x_i = x_0 + i\Delta$, and write a finite difference version of the SE by putting

$$\left.\frac{dy}{dx}\right|_{x_i} \simeq \frac{y_{i+1} - y_i}{\Delta}$$

and solve it for given V'.

(a) Make plot of a wavefunction corresponding to your first energy guess $V' = 0.8$. Is this a valid wavefunction for a particle in a box? If not, what do you have to adjust to make it a valid wavefunction?

(b) Plot first five lowest energy wavefunctions and compare with the analytical solutions.