## Multiscale Modeling and Methods Problem Set 4 by Afrina Asad Meghla

(Out Mon 10/14/2024, Due Mon 10/21/2024)

## Problem 1

Consider the time-independent Schrödinger equation for a particle in a 1D potential well is given by:

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

where V(x) is the potential,  $\hbar$  is the reduced Planck's constant, m is the mass of the particle, and E is the energy eigenvalue.

(a) The potential for this system is:

$$V(x) = \begin{cases} 0, & -L < x < L \\ \infty, & \text{otherwise} \end{cases}$$

where L is the half width of the well.

Derive the equation for wavefunction and eigenvalue for the well for symmetric case.

**Ans:** The expected energy level(eigenvalue):  $E_n = \frac{n^2 \pi^2 \hbar^2}{8mL^2}$ (b) Now Consider this potential for the system:

$$V(x) = \begin{cases} 0, & -L < x < L \\ V_0, & \text{otherwise} \end{cases}$$

Derive the wavefunctions considering they need to be continuous and smooth on the boundary for symmetric case.

Your expected general form of solution for eigenfunctions:

- $\psi_1 = Ce^{\alpha x}$  (while, x < -L)
- $\psi_2 = A\sin(kx) + B\cos(kx)$  (while, -L < x < L)
- $\psi_3 = De^{-\alpha x}$  (while, x > L)

Now plot the eigenvalues since in this case they cannot be solved analytically.

**Hint**: Take  $u = \alpha L$ , v = kL and plot for  $u^2 = u_0^2 - v^2$  and  $u = v \tan(v)$ 

(c) If  $u_0 \to \infty$ , what can you say about energy level from your solution?

## Instructions

Email your solutions (i.e., a scan or typed version of your pen-and-paper part; and programming codes in a way that they can be run by someone else) to tuq07829@temple.edu with the email subject Math 8200. Homework 4 and all the submitted filenames starting with your family name.