Complete this assignment prior to the last lecture, Monday 4 May. You may work individually, or in a group(s) for this assignment.

In this lab you'll be studying the behavior of a simple quantum mechanical system, the "particle in a box." Unlike the potential well examples you saw in lecture, this one has a perturbation applied in the form of a non-zero potential centered in the well. The potential function is given by

$$V = \begin{cases} V_1 & |x| \le \ell \\ 0 & \ell < |x| \le L \\ V_o & |x| > L. \end{cases}$$

For $V_o \gg E$ and $V_1 = 0$, this is just the unperturbed square well we discussed in lecture. The solutions for the wavefunction, $\psi(x)$, are similar to the standing waves for a string of length 2L, with a normalized[1] energy spectrum given by

$$E = \pi^2 \begin{cases} \frac{1}{8}, \frac{9}{8}, \frac{25}{8}, \cdots, \frac{(2n-1)^2}{8} & E_{\text{even}} \\ \\ \frac{1}{2}, \frac{4}{2}, \frac{9}{2}, \cdots, \frac{n^2}{2} & E_{\text{odd}}. \end{cases}$$

With or without the perturbation, this potential satisfies $V(x) = V(-x)$, so there exist states of definite parity, which allows us to use the shooting method to find an approximate numerical solution for the wavefunction, $\psi(x)$.

If we let $V_1 \neq 0$, the energy spectrum for the ideal case, $V_o, V_1 \gg E$ and $\ell = L/10$, is changed to

$$E = \pi^2 \begin{cases} \frac{50}{81}, \frac{450}{81}, \frac{1250}{81}, \cdots, \frac{50(2n-1)^2}{81} & E_{\text{even-even}} \\ \\ \frac{200}{81}, \frac{800}{81}, \frac{1800}{81}, \cdots, \frac{200n^2}{81} & E_{\text{even-odd}} \\ \\ \frac{1}{2}, \frac{4}{2}, \frac{9}{2}, \cdots, \frac{n^2}{2} & E_{\text{odd}}. \end{cases}$$

Note that the even solutions now behave as two separate wells of width 9L/10, yet the odd solutions remain unchanged in energy. The reason for this is something you will have to explain.

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[1] Normalized units such that $L = \hbar = m = 1$.

In this lab you'll numerically examine a more realistic case: $V_o \gg V_1 > E$. Since V_1 is finite, there will be departures from the shifted energy spectrum, above. Your job is to describe those departures.

Using the techniques we discussed in class and my MATLAB visualization function, you'll calculate the ground state and first three excited state energies for this potential function given the following conditions

- Normalized units such that $L = \hbar = m = 1$
- $\Delta x = 10^{-3}$
- $\ell = L/10$
- $V_o = 10^5$
- $V_1 = 10^2$
- and let your initial conditions for ψ be given by

$$\psi_{\text{even}}(-\Delta x) = 0.04 \qquad \psi_{\text{odd}}(-\Delta x) = -\Delta x$$
$$\psi_{\text{even}}(0) = 0.04 \qquad \psi_{\text{odd}}(0) = 0.$$

You'll only need to solve for $\psi(x)$ in the region $x \in [0, L + \kappa]$, since my plot function will unfold your solution for $x < 0$. Let $\kappa \sim 0.2L$ for a robust solution. See the function for details.

Answers to the following questions and the following products should comprise your submission for this lab.

1. Plot the ground state and first three excited states using my MATLAB visualization function.
2. Estimate the energies of each of those states and compare to the ideal case. What has happened to each?
3. Why are the energies associated with the ideal even wavefunctions representative of of two smaller wells, while the ideal odd wavefunction energies are not?