PHYS 305: Computational Physics II

Winter 2022

Homework #5

(Due: March 5, 2022)

Each problem is worth 10 points. Upload your solutions to Learn with a title including PHYS 305 and the Homework number. The PDF upload should contain all discussion, results, and graphs requested, and files containing Python scripts for all programs written.

1. Do Exercise 7.3 on the course web site.

2. Extend the finite-well calculation carried out in class as follows. In scaled units, Schrödinger's equation is

$$-\frac{d^2\psi}{dx^2} = (z - U)\,\psi\,,$$

where

$$U = \begin{cases} 0 & (|x| < 1)\,, \\ U_0 & (|x| > 1)\,. \end{cases}$$

We will search for even and odd solutions separately. We shoot from the center ($x = 0$) to the edge ($x = 1$) of the well.

For even solutions, the central boundary conditions are $\psi(0) = 1, \psi'(0) = 0$ (we can always scale ψ to satisfy the normalization condition). For odd solutions, we take $\psi(0) = 0, \psi'(0) = 1$. The boundary condition at $x = 1$ is that the solution match smoothly onto the exterior solution $\psi \sim e^{-\eta x}$ (with η as defined in class: $\eta^2 = U_0 - z$), so $\psi' + \eta\psi = 0$ at $s = 1$. The free variable z is the scaled energy; the error is $g(z) = \psi'(1) + \eta\psi(1)$.

For any choice of U_0, find <u>all</u> bound solutions. Then, by looping over U_0, for $U_0 = 0, \ldots, 100$ in steps of 0.1, plot your solutions for the scaled energy z as functions of scaled potential U_0.

3. Find the first 10 energy eigenvalues and eigenfunctions of the harmonic oscillator with

$$U(x) = x^2$$

by shooting from $x = 0$ to $x = x_0 = 6$ and assuming $\psi(x_0) = 0$. Be sure to include both even and odd solutions. Plot all eigenfunction solutions on a single graph, clearly indicating the energies associated with each.

What happens to the eigenvalues and eigenfunctions you calculate if x_0 is reduced to 4?

4. Find all bound solutions of the Schrödinger equation with potential

$$U(x) = -e^{-|x|^{1/2}}.$$

Plot the eigenfunctions and state the eigenvalues.