PHYS 307: Computational Physics Lab (QM)

Winter 2012

Homework #3

(Due: February 13, 2012)

1. Use the programs written in class to solve numerically the differential equation

$$\frac{d^2y}{dx^2} = f(x, y, y'),$$

on the interval $a \leq x \leq b$, subject to the boundary conditions

$$y(a) = \alpha, \quad y(b) = \beta.$$

Use steps of $\delta x = (b-a)/200$ in the integrator, and solve the resulting equation to a tolerance of $\epsilon = 10^{-4}$.

Specifically, solve the following problems:

(a) $a = 0,\ b = 1,\ f(x, y, y') = -y^2,\ \alpha = 1,\ \beta = 0.5$,

(b) $a = -1,\ b = 1,\ f(x, y, y') = -y' - 30y^3,\ \alpha = 2,\ \beta = -2$,

(c) $a = 0,\ b = 1,\ f(x, y, y') = e^{x+y},\ \alpha = 1,\ \beta = 0$.

In each case, print out (1) your initial guesses for $y'(a)$ bracketing the root, (2) the value of $y'(a)$ that solves the problem to the specified accuracy, and (3) the number of iterations required. By adding a print statement to the integrator, also plot your successive approximations to the solution of part (b).

As usual, turn in both your program and the results produced when it runs.

2. Repeat the calculation in Homework 2, but this time using a numerical boundary-value solver to compute the energy eigenvalues of the finite well.

Defining $s = x/a$, Schrödinger's equation becomes

$$-\frac{d^2\psi}{ds^2} = (\xi^2 - U)\,\psi,$$

where

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

in the terminology of the earlier problem. We will search for even and odd solutions separately. We shoot from the center ($s = 0$) to the edge ($s = 1$) 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 $s = 1$ is that the solution match smoothly onto the exterior solution $\psi \sim e^{-\eta s}$ (with η as defined in Problem 1), so $\psi' + \eta\psi = 0$ at $s = 1$. The free variable (z in our classroom discussion) is ξ^2, the scaled energy; the error is $g(z) = \psi'(1) + \eta\psi(1)$.

As in Homework 2, plot your solutions for scaled energy ξ^2 as functions of scaled potential U_0, for $U_0 = 0, \ldots, 100$ in steps of 0.1. Turn in your final program, as well as a graph of $\xi^2(U_0)$ for $0 \leq U_0 \leq 100$.