Name: ____________________, ____________________

PHYSICS 401 : SPRING SEMESTER 2018

Project #8: Solving the radial Schrödinger equation

1. Use the second order Verlet method as presented in class to solve for the eigenvalues of the hydrogen atom with potential $V(r) = -1/r$. Working in atomic units (length in Bohr radus and energy in Hartree, (1/2)Hartree =13.6 ev) corresponding to setting $\hbar^2/m = 1$. To compute the first few eigenvalues of each angular momentum $\ell = 0, 1, 2, 3$, use the following artificial hard wall method. Let's pretend that the nucleus is fixed at the origin and is enclosed by an infinite spherical wall at $r = C$. That is, the radial wavefunction must obey the condition $u(r = C) = 0$. First, pick $\ell = 0$ and construct a do-loop to systematical increases the energy e from -1 to 0 (spanning the entire spectrum of the hydrogen atom) in steps of 0.001. At each value of e, starting at the origin, set $u(0) = u_0 = 0.0$, $dr = 0.01$, $u_1 = u(dr) = 0.01$, $u_n = u(n * dr)$, and integrate the radial wavefunction out to $r = 25$ (use double precision). Whenever the wave function crosses zero, (that is, whenever $u_n * u_{n-1} < 0$) output the energy e and the value $r = n * dr$ (=C). Repeat this for $\ell = 1, 2, 3$. Plot the graph of e vs C using different plotting symbols for $\ell = 0, 1, 2, 3$. What are the energies in this graph correspond to? Where are the energies of the hydrogen atom? ($e_n = -1/(2n^2)$), where n here is the principle quantum number).

2. Determine the value of π to ≈ 14 digits by solving for the root of the equation

$$f(x) = \cos(x) = 0$$

using the second order Newton's method. The exact solution is $x^* = \pi/2$, so that $\pi = 2x^*$. Use the initial guess of $x = 1.5$, corresponds to a guess of $\pi \approx 3$. How many iterations are needed to achieve 14 digits? Repeat the calculation with initial guesses $x = 1$, $x = 0.5$ and $x = 0.25$.

3. Use the Killingbeck method as presented in class to solve for the eigenvalues of the hydrogen atom as in 1), but with greater accuaracy. Use the same Verlet algorithm to integrate backward to the origin from r = 25. Do Newton's iterations 4-10 times to find the correct ϵ so that $u(0, \epsilon) = 0$. Determine the lowest energy levels of $\ell = 0, 1, 2, 3$. Use $\epsilon = -0.6$ as your initial guess energy. Plot all energy values as a function of dr from 0.01 to 0.1.