PHYS 305: Computational Physics II

Winter 2022

Homework #6

(Due: March 13, 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. (a) Use the basic matrix method to find the first 10 energy eigenvalues and eigenfunctions of the harmonic oscillator with
$$U(x) = x^2$$
on the range $-x_0 \le x \le x_0$, with $x_0 = 6$ and assuming $\psi(\pm x_0) = 0$. Plot all eigenfunction solutions on a single graph, clearly indicating the energies associated with each. The analytic solution for the energy of the n-th eigenstate is $E_n = 2n + 1$. How many grid points are needed to ensure that the numerical solutions are all within 10^{-4} of the analytic results?

   (b) Repeat part (a) using the Numerov method.

2. Use the Numerov method to find the 4 lowest energy solutions of the Schrödinger equation with potential
$$U(x) = -e^{-|x|^{1/2}}.$$
Plot the eigenfunctions and state the eigenvalues. Note that, since $U \to 0$ as $x \to \infty$, we expect the wavefunction to go exponentially to zero like $e^{-|E|^{1/2}x}$. If your wavefunction has any significantly nonzero slope at the ends of the x range you choose, you will have to make the range larger. What range and how many grid points do you need to adequately determine the 4 wavefunctions you obtain?

3. The wavefunction of a hydrogen atom obeys the 3-dimensional Schrödinger equation and, after the angular component has been decomposed into spherical harmonics, the equation for the radial part $R(r)$ is
$$\frac{d}{dr}\left(r^2 \frac{dR}{dr}\right) - \frac{2m_e r^2}{\hbar^2}\left[V(r) - E\right] R = l(l+1)R,$$
where $V(r) = -e^2/4\pi\epsilon_0 r$ and l is the angular momentum quantum number. Writing $u = rR$, it is easily shown that the equation becomes
$$\frac{d^2u}{dr^2} + \frac{2m_e}{\hbar^2}\left(\frac{e^2}{4\pi\epsilon_0 r} + E\right) u = l(l+1)\frac{u}{r^2}.$$
Now rescale the equation, writing $x = r/a_0$, where $a_0 = 4\pi\epsilon_0\hbar^2/m_e e^2$, to find
$$\frac{d^2u}{dx^2} + \left(\frac{1}{x} + \frac{E}{E_0}\right) u = l(l+1)\frac{u}{x^2},$$

where $E_0 = m_e e^4/2h^2\epsilon_0^2 = 4$ Ry $= 54.4$ eV.

Use the Numerov method to find the 4 lowest energy states of this system for $l = 0$ and $l = 1$. For each value of l, plot all 4 wavefunctions on the same graph. Take $u(0) = 0$ and $u(x_m) = 0$, where x_m is chosen so that the solution is clearly going exponentially to zero.