Spring 2021
PHYS 377 Advanced Computational Physics
HW # 5b

<u>Problem 1:</u> Quantum oscillators

Consider the 1-D, time-independent Schrödinger equation in a harmonic (*i.e.* quadratic) potential $V(x) = V_0 x^2/a^2$, where V_0 and a are constants.

(a) (80 points) Write down the **Schrödinger equation** for this problem and convert it from a *second-order* equation to two *first-order* equations. **Write a program** to find the energies of the ground state and the first two excited states for these equations when m is the electron mass, $V_0 = 50$ eV, and $a = 10^{-11}$ m. Note that in theory the wavefunction goes all the way out to $x = \pm\infty$, but you can get good answers by using a large but finite interval. Try using $x = -10a$ to $+10a$, with the wavefunction $\psi = 0$ at both boundaries. (In effect, you are putting the harmonic oscillator in a box with impenetrable walls.) The wavefunction is real everywhere, so you don't need to use complex variables, and you can use evenly spaced points for the solution.

The quantum harmonic oscillator is known to have energy states that are equally spaced. Check that this is true, to the precision of your calculation, for your answers. (Hint: The ground state has energy in the range 100 to 200 eV.)

(b) (10 points) Now **modify your program** to calculate the same three energies for the anharmonic oscillator with $V(x) = V_0 x^4/a^4$, with the same parameter values.

(c) (10 points) **Modify your program** further to calculate the properly normalized wavefunctions of the anharmonic oscillator for the three states and make a plot of them, all on the same axes, as a function of x over a modest range near the origin—say $x = -5a$ to $x = 5a$.

To normalize the wavefunctions you will have to evaluate the integral

$$\int_{-\infty}^{\infty} |\psi(x)|^2 dx$$

then rescale ψ appropriately to ensure that the area under the square of each of the wavefunctions is 1. Either the trapezoidal rule or Simpson's rule will give you a reasonable value for the integral. Note, however, that you may find a few very large values at the end of the array holding the wavefunction. Where do these large values come from? Are they real, or spurious?

One simple way to deal with the large values is to make use of the fact that the system is symmetric about its midpoint and calculate the integral of the wavefunction over only the left-hand half of the system, then double the result. This neatly misses out the large values.