Chem 302 Laboratory 3

Numerically Solving The Schrodinger Equation for

Harmonic and Anharmonic Oscillator Wave Functions

NAME:

1. What is the Schrodinger equation for a 1D harmonic oscillator? Identify the Kinetic and Potential energy operators.
2. Using the **Numerov.functions.R** and **Numerov\_control.R** scripts, initialize the correct potential and solve this differential equation for over a stretching domain of -5 Å to 5 Å. Do this for the ground, first, second, third and fourth excited states. Upload plots of your wave functions. Write down the eigenvalues you obtain.
3. What is the energetic difference between each adjacent pair of energies. Do the results make sense? Why?
4. Using the **Numerov.functions.R** and **Numerov\_control.R** scripts, plot the anharmonic potential over a stretching domain of -0.8 Å to 5 Å making sure that the well is clearly visible. Upload your plot.

Using the **Numerov.functions.R** and **Numerov\_control.R** scripts, and the anhamonic potential above, solve the Schrodinger equation for the ground, first and second excited states. Normalize the wave functions and upload their plots. Write down the eigenvalues you obtain.

1. Compute and plot the 16th and 17th excited state wave functions for the anharmonic oscillator (Don’t bother to try and normalize it). HINT: You will have to modify the right side of the stretching domain. These wave functions will be pretty high in energy and will require a long x-axis. Set x.max to about 14.5 or 15 at least. Write down the eigenvalues you obtain.

As we can see the right side of the seventeenth excited state wave function is a bit wild and will not form a decaying tail. What may be going on?