Chem 302 Laboratory 3

Numerically Solving The Schrodinger Equation for

Harmonic and Anharmonic Oscillator Wave Functions

NAME:

Write down the Schrodinger equation for a 1D harmonic oscillator. Identify the Kinetic and Potential energy operators.

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. Write down the eigenvalues you obtain.

What is the energetic difference between each adjacent pair of energies. Do the results make sense? Why?

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. Print out your plot.

Using the **Numerov.functions.R** and **Numerov\_control.R** scripts, and the anhamonic potential above, solve the Schrodinger equation for the ground and first excited states. Normalize the wave functions and print out their plots.

Compute and plot the 17th excited state wave function 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. What is the explanation of the behavior you observe in the graph?

**Bonus** (5 points next exam): Use your code above in R and evaluate the integral. To get credit, you must answer all questions correctly and get the correct value for the integral. Paste in a screen shot of your R-Studio code for the integral and the value you obtain.

A curve in R is represented internally as a vector of points. If we wish to integrate this curve, the vector of points must be used to construct an R “spline” function.

a. **Define**:

interpolation

spline

spline function

b. What does the R function splinefun do? Give an R example of using the R splinefun. Explain what is going on.

c. What function in R can be used to integrate? Give an example in R code of integration.

d. Given a vector of points representing the normalized 1st excited state harmonic oscillator wave function, **1 found with the Numerov procedure, write out the R code to evaluate the integral:

e. What does this integral physically represent?