Chem 302 Laboratory 4

Numerically Solving The Schrodinger Equation for

Hydrogen Like Atoms

NAME:

1. Write down the Schrodinger equations for the radial and angular wave functions of a Hydrogen-like (one-electron) atom. Identify the kinetic and potential energy terms.
2. Using the **Numerov.functions.R** and **Numerov\_laguerre\_control.R** scripts choose a maximal radial distance and solve the radial Schrodinger equation for the 1*s* state. Plot the radial *wave function* you obtain. Indicate the nodes if there are any.
3. Repeat the above procedure for the 2*s*, 2*p* and 3*d* radial wave functions. Adjust the length of the *r*-axis as needed to see a long decaying tail to the wave function. Record how long this is for each. Also record the number of radial nodes observed in the plots. Do the number of radial nodes agree with the analytical formula?
4. Using our **Numerov.functions.R** and **Numerov\_laguerre\_control.R** scripts plot the radial part of the wave function of an electron with an orbital angular momentum magnitude of and a principal quantum number of 6.
5. Using our **density.sampling.functions.R** and **density.sampling.control\_script.R** plot the 3D electron probability density scatter plots for the 1*s*0, 2*p*-1, 3*d*0, 3*p*-1 orbitals. On your plots, indicate any angular nodal planes that may exist.