Chem 302 Laboratory 4

Numerically Solving The Schrodinger Equation for

Hydrogen Like Atoms

NAME:

1. Using the **Numerov.functions.R** and **Numerov\_laguerre\_control.R** scripts choose a reasonable maximal radial distance (to show the right tail) and solve the radial Schrodinger equation for the 1*s* state. Plot the **normalized** radial *wave function* you obtain. Record the number of nodes.
2. 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 the number of radial nodes observed in the plots.
3. Using our **Numerov.functions.R** and **Numerov\_laguerre\_control.R** scripts plot the **normalized** radial part of the wave function of an electron with an orbital angular momentum magnitude of and a principal quantum number of 6. What is the orbital angular momentum letter (*i.e.* s, p, d, f, g, …)?
4. 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. Indicate the eigenvalue and number of angular nodal planes that for each orbital.
5. The highest atomic number and highest atomic mass element yet synthesized is Oganesson (118Os). Though extremely short lived, it is in the noble group of the periodic table and expected to fully fill it’s 7p subshell (predicted electron configuration: [Rn]5f14 6d10 7s2 7p6). Compute and plot the normalized radial wave function for the 7p subshell. Record the number of radial nodes and the magnitude of the orbital angular momentum for an electron in this subshell. Finally, plot a 7p probability density scatter plot and record the number of angular nodes.