



Mathematica Exercise: One-electron Atomic Wavefunctions

*Physical Chemistry I
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The radial wavefunctions as well as the solutions for a single-electron atom can be found in Dr. Francl's Handy Guide to Quantum Mechanics. They have also been set-up in the Mathematica notebook HAtomSolnsExercise.nb. Use those functions to explore some of the common concepts about atomic orbitals that are presented in general chemistry courses. Note that the radial probability distribution is given by $(R_n(r))^2 r^2$.

1. *The principal quantum number, n , controls the size of the orbital.* Find the average distance from the nucleus ($\langle r \rangle$) for the 1s, 2s and 3s orbitals in a hydrogen atom.

2. *s orbitals have no nodes.* Plot the 1s, 2s and 3s radial distribution functions for a hydrogen atom. How many nodes would a 5s orbital have?

3. *Which is larger (extends further from the nucleus), a 2s or a 2p orbital?* Make a prediction, then compare the average distance from the nucleus ($\langle r \rangle$) for the 2s and 2p, and the 3s and 3p orbitals in a hydrogen atom.

4. *Which is larger, the 2s orbital in C^{5+} or the 2s orbital in Li^{2+} ?* Make prediction, then compute the average distance from the nucleus for both functions. Does the answer surprise you?

5. I have some commands to make contour plots of the orbitals at the end of the notebook. Why did I chose the functions I did to plot?