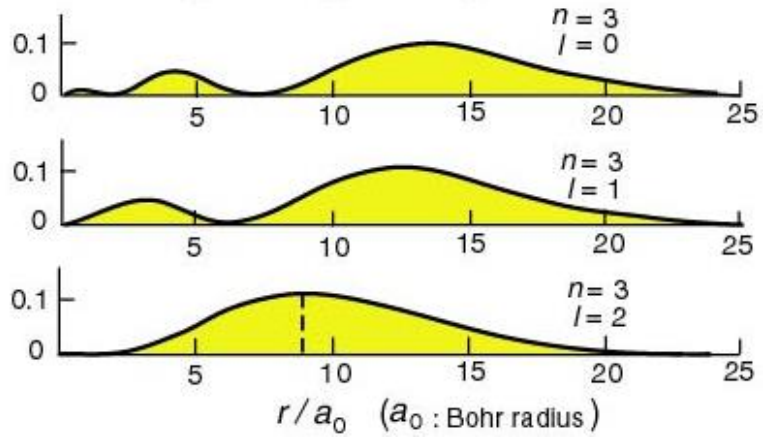
Problem set 3

1. The radial distribution function (RDF), P(r), for the 1s orbital is defined as:
   $P_{1s}(r) = 4\pi r^2 [\psi_{1s}(r)]^2$
   For an electron in a 1s orbital, how does the RDF vary with distance from the nucleus? Explain why it is that although the 1s wavefunction is a maximum at the nucleus, the corresponding RDF goes to zero at the nucleus. Also, explain why the RDF shows a maximum, and why the RDF goes to zero for large values of the distance r.

2. In a single graph with proper axes labels, draw the Radial Function for 1s,2s,2p and in another graph draw for 3s, 3p, 3d orbitals for a Hydrogen atom indicating nodes and relative position of the maxima. Repeat the same exercise for the Radial Distribution Function. Qualitatively explain what happens in case of the other hydrogenic atoms such as Li^{+2}?

3. The Radial Distribution Function of 3s, 3p and 3d is given below.



   (i) In which of the orbitals is the highest probability of finding electron [indicated by the maxima of $P_{1s}(r)$] closest to the nucleus
   (ii) If you consider distance of $0.1a_0$ from the nucleus, in which of the three orbitals would you have the maximum probability of finding electrons.

4. What do you understand by the terms radial node and nodal plane, as applied to AO wavefunctions? Illustrate your answer using the 2s and 2p AOs. Explain why radial nodes arise from the radial part of the wavefunction, whereas nodal planes arise from the angular part of the wavefunction.

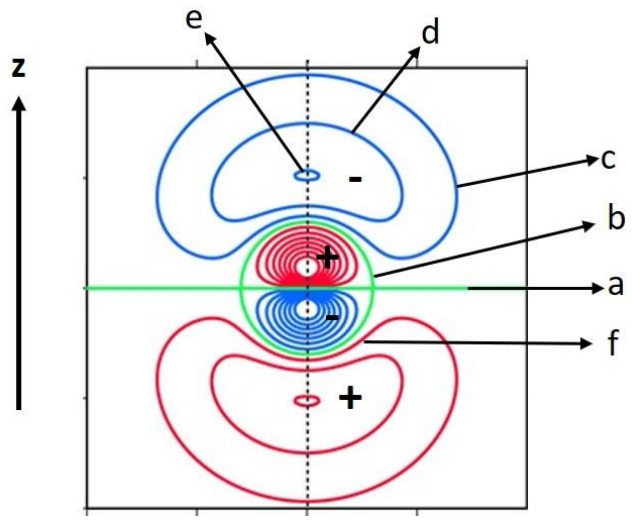
5. The radial part of the 3p AO wave function is:

$$R_{3,1}(r) = N_{3,1}\left[6\left(\frac{r}{a_0}\right) - \left(\frac{r}{a_0}\right)^2\right]\exp\left(-\frac{r}{3a_0}\right).$$

Determine the position of the radial node in the 3p orbital?

6. Draw up a table showing the number of radial nodes, the number of angular nodes (nodal planes), and the total number of radial and angular nodes for 1s, 2s, 2p, 3s and 3p orbitals.

7. The contour plot of wavefunction (ψ) shown below is of one of the p orbitals: positive intensity is indicated by red contours, negative by blue, and the zero contour is indicated in green.



(i) Which p orbital is represented by this contour plot.
(ii) What does "a" and "b" represent?
Consider that the contour plot of ψ^2 looks like the plot shown above (of course, there will be no "signs"). In such a scenario:
(iii) What would each line (red/blue) in the contour plot indicate?
(iii) Between "c", "d" and "e", rank them in the increasing order of "probability of finding electrons"
(iv) Between points "d" and "f" which represents the higher probability of finding electrons

8. Sketch 3s, 2p and 3p orbitals using only one surface of the contour plot as taught in class. E.g.: the plot for 2s will be like: