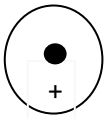
Problem Set 3

1. Sketch the 2s, 3s and 4s orbitals of H-atom (draw only one equal probability iso-surface; NOT contour plots, e.g., 1s should be sketched as shown below). Label the axis, nucleus, radial node, nodal plane and sign of wavefunction, wherever applicable.

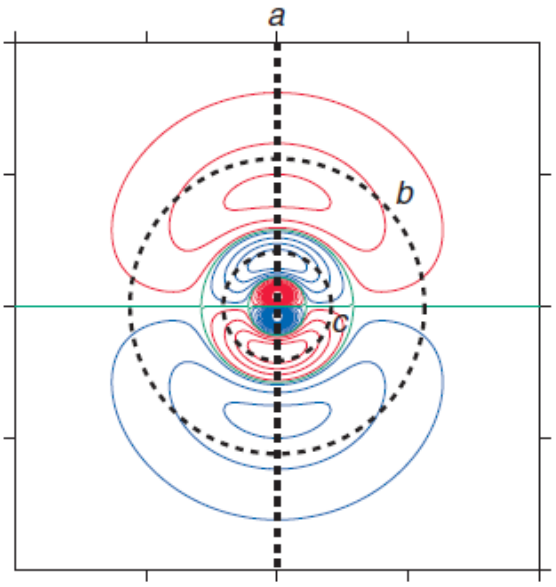


2. Sketch the $2p_x$, $3p_z$ and $4p_y$ (draw only one equal probability iso-surface; NOT contour plots). Label the axis, nucleus, radial node, nodal plane and sign of wavefunction, wherever applicable.

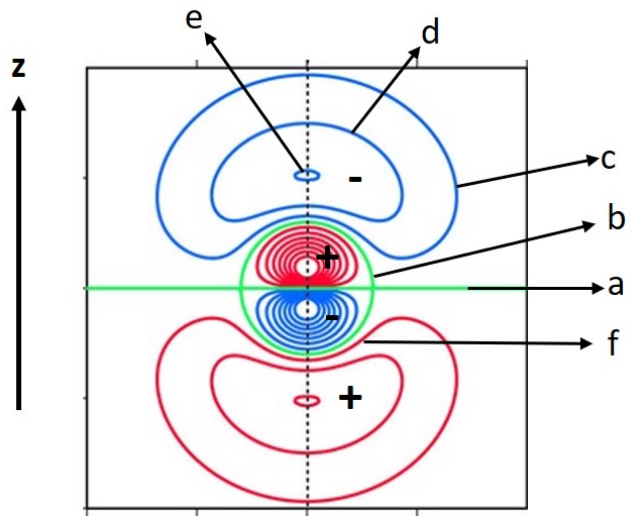
3. Draw up a table showing the number of radial nodes, the number of angular nodes (nodal planes), and the total number of radial and angular nodes for 1s, 2s, 2p, 3s and 3p orbitals.

4. For the Li atom, compare the 2s and 2p electrons in terms of shielding ability? Explain.

5. The contour plot shown below is of one of the 4p orbitals: positive intensity is indicated by red contours, negative by blue, and the zero contour is indicated in green.
Sketch how the wavefunction will vary along the dotted line a, and along the two circular paths b and c (for the latter two, this means making a plot of the wavefunction as a function of an angle which specifies how far we have moved around the circle).



6. The contour plot of wavefunction (ψ) shown below is of one of the p orbitals. Consider that the contour plot of ψ^2 looks like the plot shown below (of course, there will be no "signs"). In such a scenario, which of the following statements is true:



(A) Between “c”, “d” and “e”, the “probability of finding electrons” increases in the order c>d>e

(B) The circle “b” represents the angular node

(C) The line “a” represents the radial node

(D) The “probability of finding electrons” is higher in the point “d” in comparison to “f”