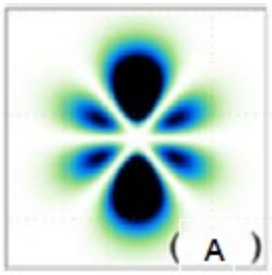
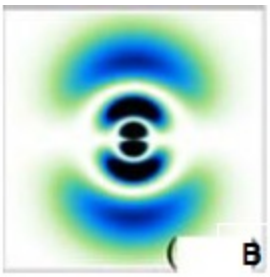
CH-107 Tutorial-3

1. **Sketch the polar plot of dz2 orbital as a function of θ and ϕ. Pictorially, depict the angular nodes present for $3d_{z^2}$ orbital of hydrogen atom [$3d_{z^2} = N_1(r/a_0)^2(3\cos^2\theta - 1)e^{-r/3a_0}$]. How many nodal planes/surfaces are present and at what values of (r,θ,ϕ)?**

2. **From the projections of the hydrogenic orbitals shown below, guess the quantum numbers n and l. Assign a sign to regions and show radial/angular nodes for each orbital. (Vertical direction: z-axis)**





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

4. **Where is the probability of finding an electron in 1s and $2p_z$ orbital greatest?**

5. **Write general Hamiltonians for a many electron atom and expand it for Li and C atoms.**

6. **Why can we not exactly solve the Schrödinger equation for He atom? What is orbital approximation?**

The following problems will be dealt with in Tutorial 4, instead of Tutorial 3.

7. **What is a spin-oribital? Why are α(1)β(2) or β(1)α(2) not acceptable two electron spin-functions?**

8. **Write the total wavefunctions (space and spin) of the He atom in the ground and first excited states. Now write the total wavefunctions in the form of Slater determinants.**

9. **Show that for Li, it is impossible to have the third electron occupy the 1s orbital (when the other two electrons already reside in 1s).**