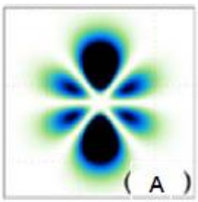
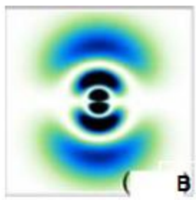
CH 107 Tutorial 4

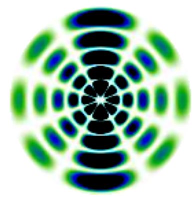
Solve these problems BEFORE the tutorial session

1. Evaluate the values of [*r, θ, φ*] for which there are radial/angular nodes (if any) for $3d_{z^2}$ orbital of H-atom? $\Psi^{320} = N\sigma^2 e^{-\sigma/3}\left(3\cos^2\theta - 1\right),\ \sigma = \dfrac{r}{a_0}$; a_0 is Bohr radius.

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. Try to guess the quantum-number m_l as well. ***Note:*** *Vertical direction: z-axis*..





(c)  (*try this just for fun* ☺)

3. In a single graph with proper axes labels, qualitatively sketch the Radial functions and Radial Distribution Functions for 1s, 2s, 2p (same graph) and 3s, 3p and 3d (same graph) orbitals for H-atom indicating nodes and relative position of the maxima/minima.

4. Why could we take a linear combination of $\psi_{2,1,+1}$ and $\psi_{2,1,-1}$ to generate two real atomic orbitals ψ_{px} and ψ_{py}? Why did not take a linear combination of $\psi_{2,1,0}$ and $\psi_{2,1,\pm1}$?

5. For which value of (*r, θ, φ*) is the probability of finding an electron in a) 1s and b) $2p_z$ orbital the greatest?

   (i) $\Psi_{1S} = 2\left(1/a_0\right)^{3/2}\exp\left(-r/a_0\right)$; (ii) $\Psi_{2P_z} = \left(1/32\pi\right)^{1/2}\left(1/a_0\right)^{5/2}\cdot r\cdot\exp\left(-r/2a_0\right)\cdot Cos\theta$

Additional questions (6-7) for you to solve: these will not be covered in tutorials!

6. Consider the following orbitals for hydrogen atom:

$$\psi_1 = \frac{1}{81}\left(\frac{1}{\pi a_0^3}\right)^{1/2}\left(\frac{r}{a_0}\right)^2 e^{-r/3a_0}\,\mathrm{Cos}\theta\mathrm{Sin}\,\theta e^{i\phi}\ ;\ \psi_2 = \frac{1}{81}\left(\frac{1}{\pi a_0^3}\right)^{1/2}\left(\frac{r}{a_0}\right)^2 e^{-r/3a_0}\,\mathrm{Cos}\theta\mathrm{Sin}\,\theta e^{-i\phi}$$

(i) Convert these two eigenstates to two new ***real*** orbitals. What are the value of *m* for the real orbitals? Express the real orbitals as *f*(*r*).*F*(*x,y,z*), and hence identify it.

7) Consider a H-atom with an electron in the 2s orbital. Calculate the probability of finding the electron in the volume defined by {5.22Å < *r* < 5.26Å}, {(½)π - 0.01 < *φ* < (½)π + 0.01}, {(½)π - 0.01 < *ϑ* < (½)π + 0.01}. Assume the *wavefunction is constant* within this volume and a_0 = 0.5 Å. (*Find out the wavefunction of 2s orbital from a book or internet*)