CH 107 Tutorial 4

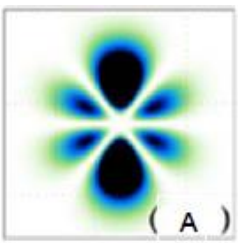
Solve these problems BEFORE the tutorial session

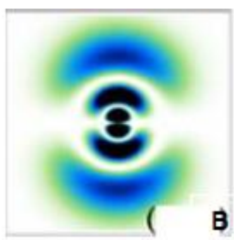
1. a) Evaluate the normalization constant *N* for the ground state wave function of hydrogen atom. $\Psi_{1s}(r,\theta,\phi) = N \exp\left(\frac{-r}{a_0}\right)$. If you need, use $\int x^n \cdot e^{-ax} dx = n!/a^{n+1}$

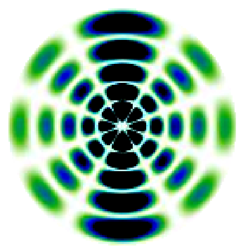
   b) For the lowest energy state of H-atom, evaluate the average distance of the electron from the nucleus.

2. Evaluate the values of [*θ, φ*] for which there are angular nodes for $3d_{z^2}$ orbital of H-atom?
   Given: $\psi_{3d_{z^2}} = N\sigma^2 e^{-\sigma/3}\left(3\cos^2\theta - 1\right) \quad \sigma = \frac{r}{a_0}$

3. 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*). Try to guess the quantum-number m_l as well.





(c)  (*try this just for fun* ☺)

4. 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.

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) $\Psi_{2P_Z} = \left(1/32\pi\right)^{1/2}\left(1/a_0\right)^{5/2} r^1 \exp\left(-r/2a_0\right) Cos\theta$

Additional questions (6-8) for you to solve: these will not be covered in tutorials!

6. a) 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 $\psi_{2,1,\pm1}$?

   b) What is the reason behind the nomenclature of the atomic orbitals such as ψ_{px}, ψ_{py}, ψ_{pz}? What is the significance of subscripts x, y and z? (Hint: *first solve Q7(ii)*)

   c) If H atom is spherically symmetric, how are $\psi_{py}, \psi_{px}, \psi_{pz}$ oriented along specific directions?

7. Consider the following orbitals for hydrogen atom (a_0 = Bohr radius):

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

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

(i) Take appropriate linear combinations of these two orbitals to generate two new real orbitals. What is the value of m_l for the two real orbitals thus generated?

(ii) Express any one of these real orbitals as $f(r).F(x,y,z)$, and hence identify the real orbital.

8) 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*)