Note Title 09-11-2016

# of radial nodes = $n - l - 1$

# of angular nodes = l

total # of nodes = $(n-l-1) + l = \underline{\underline{n-1}}$!

$n = 1, 2, 3 \ldots$

$l = 0, 1, 2, \ldots$

$m_l = 0, \pm 1, \pm 2, \ldots \pm l$

<u>Total wavefunction</u>:

$$\Psi(r, \theta, \phi) = R_{nl}(r)\, Y_{l m_l}(\theta, \phi)$$

$$\downarrow$$

$$\Psi_{n l m_l}(r, \theta, \phi)$$

$$\Psi_{100}(r, \theta, \phi) = R_{10}(r)\, Y_{00}(\theta, \phi)$$

(1s orbital)

$$\Psi_{200}(r, \theta, \phi) = R_{20}(r)\, Y_{00}(\theta, \phi)$$

Orthonormality condition

$$\int_{\text{all space}} \Psi^*_{n'l'm_l'}(r,\theta,\phi)\, \Psi_{nlm_l}(r,\theta,\phi)\, d\tau$$

$$\int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta\, d\theta \int_0^{\infty} r^2 dr\, \Psi^*_{n'l'm_l'} \Psi_{nlm_l}$$

$$= \delta_{n'n}\, \delta_{l'l}\, \delta_{m_l' m_l}$$

$$= 1 \quad ; \quad n = n';\ l = l';\ m_l = m_l'$$

$$= 0 \quad ; \text{ if any of these are not equal}$$

$$n \neq n' \text{ or } l \neq l' \text{ or } m_l \neq m_l'$$

Radial Distribution function (RDF)

$$\Psi_{nlm_l}(r,\theta,\phi) = \left[R_{nl}(r) \right] Y_{lm_l}(\theta,\phi)$$

$$\int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta\, d\theta\ \Psi^*_{nlm_l} \Psi_{nlm_l}\, r^2 dr$$

$$\left[R_{nl}(r) \right]^2 r^2 dr\ \underbrace{\int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta\, d\theta\ Y^*_{lm_l} Y_{lm_l}}_{=1 \text{ (normalisation of spherical harmonics)}}$$

$$\underbrace{[R_{nl}(r)]^2 r^2}_{P(r)} dr$$

$$RDF \equiv P(r)\,dr$$

$$P(r) = [R_{nl}(r)]^2 r^2$$

<u>Specific case</u> <u>1s orbital</u>

$$\psi_{100}(r,\theta,\phi) = R_{10}(r)\, Y_{00}(\theta,\phi)$$

$$R_{10}(r) = \left(\frac{Z}{a_0}\right)^{3/2} \exp(-\rho/2)\, 2$$

$$Y_{00} = \frac{1}{\sqrt{4\pi}}$$

$$\psi_{1s} \equiv \psi_{100} = 2\frac{1}{\sqrt{4\pi}}\left(\frac{Z}{a_0}\right)^{3/2} \exp(-\rho/2)$$

<u>Z=1</u>

<u>H-atom</u>

$$\psi_{100} = \frac{1}{\sqrt{\pi}}\left(\frac{1}{a_0}\right)^{3/2} \exp\left(-\frac{2Zr}{na_0}\frac{1}{2}\right)$$

$$\psi_{100} = \frac{1}{\sqrt{\pi}}\left(\frac{1}{a_0}\right)^{3/2} \exp\left(-\frac{r}{a_0}\right)$$

$$\underline{\psi_{1s} = \left(\frac{1}{\pi a_0^3}\right)^{1/2} \exp\left(-\frac{r}{a_0}\right)}$$

What is the most probable distance of the e^- from the nucleus in the 1s-orbital

$$P(r) = [R_{nl}(r)]^2 r^2$$

$$\frac{dP(r)}{dr} \Rightarrow$$

$$[R_{nl}(r)]^2 = [R_{10}(r)]^2$$

$$P(r) = [R_{10}(r)]^2 r^2$$

$$= \left[2\left(\frac{Z}{a_0}\right)^{3/2} \exp(-\rho/2)\right]^2 r^2$$

$Z = 1$

$$= \left\{\frac{4}{a_0^3}\left\{\exp\left(-\frac{2Zr}{na_0}\cdot\frac{1}{2}\right)\right\}^2\right\} r^2$$

$$P(r) = \frac{4}{a_0^3}\exp\left(-\frac{2r}{a_0}\right) r^2$$

$$\frac{dP(r)}{dr} = \frac{4}{a_0^3}\frac{d}{dr}\left[r^2 e^{-2r/a_0}\right]$$

$$= \frac{4}{a_0^3}\left[2re^{-\frac{2r}{a_0}} - \frac{2r^2}{a_0}e^{-2r/a_0}\right]$$

$$= \frac{4}{a_0^3}2e^{-2r/a_0}\left[r - \frac{r^2}{a_0}\right] = 0$$

$$r = a_0 = r_{mp}$$

Hydrogen like atom ; $r_{mp} = \frac{a_0}{Z}$

Atomic Spectra :

Selection rules :

$\Delta l = \pm 1$; $\Delta m_l = 0, \pm 1$

no restriction is imposed on Δn

4d orbital $\rightarrow$ $l = 2$

$$l = 2 \begin{cases} \rightarrow l = 3 \quad (nf) \\ \rightarrow l = 1 \quad (np) \end{cases} \Bigg\} \ \Delta m_l = 0, \pm 1$$