Nodes

of radial nodes $= n - l - 1$

# of angular nodes $= l$

total # of nodes $= n - 1$

Total wavefunction

$$\psi_{n l m_l}(r, \theta, \phi) = R_{nl}(r)\, Y_{l m_l}(\theta, \phi) \quad \ldots (1)$$

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

(1s orbital)

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

(2s orbital)

$$\psi_{210}(r, \theta, \phi) = R_{21}(r)\, Y_{10}(\theta, \phi)$$

Orthonormality

$$\int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta\, d\theta \int_0^{\infty} r^2 dr\, \psi^*_{n' l' m_l'}(r, \theta, \phi)\, \psi_{n l m_l}(r, \theta, \phi)$$

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

$= 1$ if $n' = n,\ l' = l,\ m_l' = m_l$

$= 0$ if either $n' \neq n$ or $l' \neq l$ or $m_l' \neq m_l$

Radial Distribution Function (RDF)

$$\psi_{nlm_l}(r,\theta,\phi) = R_{nl}(r)\, Y_{lm_l}(\theta,\phi)$$

$$\int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta\, d\theta\; \psi^*_{nlm_l}\, \psi_{nlm_l}\, r^2\, dr$$

$$= \int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta\, d\theta\, [R_{nl}(r)]^2\, Y^*_{lm_l} Y_{lm_l}\, r^2\, dr$$

$$= [R_{nl}(r)]^2 r^2 dr \underbrace{\int_0^{2\pi} d\phi \int_0^{\pi} \sin\theta\, d\theta\; Y^*_{lm_l} Y_{lm_l}}_{=1}$$

(normalisation condition of Spherical harmonics)

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

$$= P(r)\, dr \quad ; \quad P(r) = [R_{nl}(r)]^2 r^2$$

1s orbital

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

$$\psi_{100} = \left(\frac{Z}{a_0}\right)^{3/2} e^{-\rho_n/2}\, 2\, \frac{1}{\sqrt{4\pi}}$$

$$\rho_n = \frac{2Zr}{na_0}$$

H-atom (1s orbital) $\Rightarrow Z = 1$

$$\Psi_{100} = 2\left(\frac{1}{a_0}\right)^{3/2} \frac{1}{\sqrt{4\pi}} e^{-\frac{2Zr}{a_0}\cdot\frac{1}{2}}$$

$$\underline{\Psi_{100} = \left(\frac{1}{\pi a_0^3}\right)^{1/2} e^{-r/a_0}}$$

Total wavefn. of the 1s-orbital
of the H-atom

$$P(r) = \left[R_{nl}(r)\right]^2 r^2 \quad \text{for H 1s-orbital}$$

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

$$= \left[\frac{4}{a_0^3}\right]\left[e^{-\frac{2Zr}{na_0}\cdot\frac{1}{2}}\right]^2 r^2$$

$$= \frac{4}{a_0^3} e^{-\frac{2r}{a_0}} r^2$$

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

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

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

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

$$= \frac{4}{a_0^3} e^{-2r/a_0}\, 2r\left[1 - \frac{r}{a_0}\right]$$

equating $\frac{dP(r)}{dr} = 0$

$$\Rightarrow \quad \underline{\underline{r = a_0}}$$

$$\underline{r_{mp} = a_0}$$

for any Hydrogenic atom $\quad \underline{r_{mp} = \frac{a_0}{Z}}$