

Que. \rightarrow . obtain the value of angular wave function $\Theta_{l,m}(\theta)$ for dxz orbital.

Solⁿ \rightarrow . since for dxz -orbital,

$$l = 2, m = +1$$

$$2l+1 = 2 \times 2 + 1 = 5$$

$$l+m = 2+1 = 3$$

$$l-m = 2-1 = 1$$

$$\Theta_{l,m}(\theta) = B P_l^m(\cos\theta)$$

where

$$B = \left[\frac{(2l+1)(l-m)!}{2(l+m)!} \right]^{1/2}$$

$$= \left[\frac{5 \times 1!}{2 \times 3!} \right]^{1/2}$$

$$= \left[\frac{5 \times 1}{2 \times 3 \times 2} \right]^{1/2} = \sqrt{5/12}$$

$$B = \sqrt{5/12}$$

$$P_l^m = \frac{1}{2^l \cdot l!} (1 - \cos^2\theta)^{m/2} \times \frac{d^{l+m}}{d(\cos\theta)^{l+m}} (\cos^2\theta - 1)^l$$

$$= \frac{1}{2^2 \cdot 2!} (1 - \cos^2\theta)^{1/2} \cdot \frac{d^3}{d(\cos\theta)^3} (\cos^2\theta - 1)^2$$

$$= \frac{1}{8} (\sin^2\theta)^{1/2} \cdot \frac{d^3}{d^3 \cos\theta} (\cos^4\theta + 1 - 2\cos^2\theta)$$

$$= \frac{1}{8} (\sin^2\theta)^{1/2} \frac{d^2}{d^2 \cos\theta} (4\cos^3\theta + 0 - 4\cos\theta)$$

$$= \frac{1}{8} (\sin^2\theta)^{1/2} \frac{d}{d \cos\theta} (12\cos^2\theta - 4)$$

$$P_l^m = 3 \sin \theta \cos \theta$$

$$\theta_{1,m}(\theta) = \theta_{2,1}(\theta)$$

$$= \sqrt{5/12} \cdot 3 \sin \theta \cos \theta$$

$$= \frac{\sqrt{15}}{4} \sin \theta \cos \theta$$

$$\left\{ \theta_{1,m}(\theta) \right\}^2 = \left\{ \theta_{2,1}(\theta) \right\}^2$$

$$= \left(\frac{\sqrt{15}}{4} \cdot \sin \theta \cos \theta \right)^2$$

$$= \frac{15}{4} \sin^2 \theta \cos^2 \theta$$

Angular probability density distribution \rightarrow

$$\int_0^\pi \theta_{1,m}^2(\theta) \sin \theta \cdot d\theta$$

$$= \int_0^\pi \frac{15}{4} \sin^2 \theta \cos^2 \theta \cdot \sin \theta \cdot d\theta$$

$$= \frac{15}{4} \int_0^\pi (1 - \cos^2 \theta) \cos^2 \theta \sin \theta \cdot d\theta$$

$$\text{let } \cos \theta = z$$

$$-\sin \theta \cdot d\theta = dz$$

$$= \frac{15}{4} \int_0^\pi (\cos^2 \theta - 1) \cos^2 \theta \sin \theta \cdot (-d\theta)$$

$$= \frac{15}{4} \int_{-1}^1 (z^2 - 1) z^2 dz$$

$$\begin{cases} \cos \theta = 1 \\ \cos \pi = -1 \end{cases}$$

$$= \frac{15}{4} \int_{-1}^1 (z^4 - z^2) dz$$

$$\Rightarrow \frac{15}{4} \left[\frac{z^5}{5} - \frac{z^3}{3} \right]_{-1}^{+1}$$

$$= \frac{15}{4} \left[\left(\frac{-1}{5} + \frac{1}{3} \right) - \left(\frac{1}{5} - \frac{1}{3} \right) \right]$$

$$= \frac{15}{4} \left[-\frac{2}{5} + \frac{2}{3} \right]$$

$$= \frac{15}{4} \times \frac{-6+10}{15} = \frac{15}{4} \times \frac{4}{15} = 1$$

∴ Angular function $\Theta_{2,1}(\theta) = \frac{15}{4} \sin^2\theta \cos\theta$ is normalised.

Q. e. ∴ The wave function for 1s-orbital is

$$\psi = \left(\frac{1}{\sqrt{\pi a_0^3}} \right) e^{-r/a_0}$$

Find the average distance of 1s electron from the nucleus.

Solⁿ. ∴

$$\langle r \rangle = \frac{\int_0^\infty \psi^* \hat{r} \psi d\tau}{\int \psi^* \psi d\tau}$$

$$= \int_0^\infty \int_0^\pi \int_0^{2\pi} \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0} \times r \times \frac{1}{\sqrt{\pi a_0^3}} e^{-r/a_0} \times r^2 \sin\theta d\theta d\phi dr$$

$$= \frac{1}{\pi a_0^3} \int_0^\infty r^3 e^{-2r/a_0} dr \times \frac{1}{\pi a_0^3} \left[\int_0^\pi \sin\theta d\theta \cdot \int_0^{2\pi} d\phi \right]$$

$$= \frac{1}{\pi a_0^3} \left[\frac{3!}{(2/a_0)^4} \cdot \left[-\cos\theta \right]_0^\pi \cdot (\phi_0)^2 \right]$$

$$= \frac{1}{\pi a_0^3} \left[\frac{3! a_0^4}{16} \times 2 \times 2\pi \right]$$

$$= \frac{3}{2} a_0 \quad \underline{\text{Ans}}$$

Que. $\therefore \rightarrow$. Calculate the most probable distance at which 1s-electron of H-like atom with atomic no. 2 is to found. Comment on the result.

Sol. $\therefore \rightarrow$.
$$\psi_{1s} = \left(\frac{z^3}{\pi a_0^3} \right)^{1/2} e^{-zr/a_0}$$

Radial distribution function

$$D = 4\pi r^2 \psi^2$$

At most probable distance

$$\left[\begin{array}{l} \psi^2 dV \\ \psi^2 d\left(\frac{4}{3}\pi r^3\right) \\ \psi^2 \frac{4}{3}\pi r^2 \end{array} \right]$$

$$\frac{dD}{dr} = 0$$

$$\frac{d}{dr} \left(4\pi r^2 \times \frac{z^3}{\pi a_0^3} \cdot e^{-2zr/a_0} \right) = 0$$

$$\text{or, } \frac{4z^3}{a_0^3} \frac{d}{dr} \left(r^2 e^{-2zr/a_0} \right) = 0$$

$$\text{or, } \frac{4z^3}{a_0^3} \left\{ e^{-2zr/a_0} \cdot 2r + r^2 \left(-\frac{2z}{a_0} \right) e^{-2zr/a_0} \right\} = 0$$

$$\text{or, } \frac{4z^3}{a_0^3} r e^{-2zr/a_0} \left(2 - \frac{2zr}{a_0} \right) = 0$$

$$\frac{4z^3}{a_0^3} r e^{-2zr/a_0} \left(2 - \frac{2zr}{a_0} \right) = 0$$

$$r \neq 0$$

$$r \neq \infty$$

$$\therefore 2 - \frac{2zr}{a_0} = 0$$

$$1 - \frac{zr}{a_0} = 0$$

$$\therefore \frac{zr}{a_0} = 1$$

$$\text{or } r = \frac{a_0}{z}$$

for H-atom

$$z = 1$$

$$\therefore r_H = \frac{a_0}{1} = a_0$$

ie: \rightarrow The normalised wave function for 1s-electron is given as

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

Calculate the probability of this electron in a sphere of radius $r = a_0$ and over all space.

solⁿ \rightarrow Probability =

$$\int_0^\infty \int_0^\pi \int_0^{2\pi} \Psi^2 d\tau$$

$$= \int_0^\infty \int_0^\pi \int_0^{2\pi} \frac{1}{\pi a_0^3} e^{-2r/a_0} r^2 dr \sin\theta d\theta d\phi$$

$$= \frac{1}{\pi a_0^3} \left[\int_0^{\infty} r^2 e^{-2r/a_0} dr \cdot \int_0^{\pi} \sin \theta d\theta \int_0^{2\pi} d\phi \right]$$

$$= \frac{1}{\pi a_0^3} \left[\frac{2!}{(2/a_0)^3} \cdot (-\cos \theta)_0^{\pi} (\phi)_0^{2\pi} \right]$$

$$= \frac{1}{\pi a_0^3} \left(\frac{2 \cdot a_0^3}{8} \times 2 \times 2\pi \right)$$

$$= 1 \text{ or } 100\% \text{ (over all space)}$$

Probability with $r = a_0$

$$= \int_0^a \psi^2 d\tau$$

$$= \frac{1}{\pi a_0^3} \left[\int_0^a r^2 e^{-2r/a_0} dr \int_0^{\pi} \sin \theta d\theta \int_0^{2\pi} d\phi \right]$$

$$= \frac{1}{\pi a_0^3} \times \frac{a_0^3}{4} (1 - 5e^{-2}) \times 2 \times 2\pi$$

$$= 1 - 5e^{-2}$$

$$e = 2.7183$$

$$e^2 = 7.3890$$

$$= 1 - \frac{5}{e^2}$$

$$= 1 - \frac{5}{7.389}$$

$$= 1 - 0.677$$

$$= 0.323 \text{ or } 32.3\%$$