Angular wave function

Que. :→. obtain the value of angular wave function $\Theta_{l,m}(\theta)$ for d_{xz} orbital.

Sol^n →. since for d_{xz} orbital.

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

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

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

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

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

where

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

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

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

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

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

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

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

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

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

$$= \frac{1}{\cancel{8}}\left(\sin^2\theta\right)^{1/2} \cdot \overset{3}{\cancel{24}}\cos\theta.$$

$$= 3\sin\theta \cdot \cos\theta$$

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

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

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

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

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

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

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

Angular probability density distribution $\mapsto$

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

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

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

Let $\cos\theta = z$

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

or, $\sin\theta \, d\theta = -dz$

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

$$= \frac{15}{4} \int_1^{-1} (z^2-1) z^2 \, dz$$

$\cos 0 = 1$

$\cos\pi = -1$

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

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

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

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

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

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

Que. :→. The wave function for 1S - orbital is

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

find the average distance of 1S electron from the nucleus.

Soln. :→.

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

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

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

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

$$= \frac{1}{\cancel{\pi a_0^3}}\left[\frac{\cancel{6}\,\cancel{a_0^4}\,a_0}{\cancel{16}}\times 2\times 2\pi\right]$$

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

Que. :→. Calculate the most probable distance at which 1S - electron of H - like atom with atomic no: Z is to found. comment on the result.

Solⁿ :→.
$$\psi_{1S} = \left(\frac{Z^3}{\pi a_0^3}\right)^{1/2} e^{-Zr/a_0}$$

Radial distribution function

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

$\psi^2 dv$
$\psi^2 d\left(\frac{4}{3}\pi r^3\right)$
$\psi^2 \frac{4}{3}\pi 3r^2$

At most probable distance

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

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

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

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

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

$$\frac{4Z^3}{a_0^3} r e^{-2Zr/a_0}\left(2-\frac{2Zr}{a_0}\right)=$$

$$r \neq 0$$

$$r \neq \infty$$

$$\therefore \quad 2-\frac{2Zr}{a_0}=0$$

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

$$\therefore \quad \frac{Zr}{a_0}=1$$

$$\text{or} \quad r=\frac{a_0}{Z}$$

for H-atom

$$Z=1$$

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

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