Que :→ Calculate the wave function, Probability density and Probability of finding the electron in the H-atom. or To show that the wave function is normalised.

Sol^n :→ For 1S-orbital,

$n = 1$

$l = 0$

$r = n+l = 1+0 = 1$

$s = 2l+1 = 2\times0+1 = 1$

$n-l-1 = 1-0-1 = 0$

$$R_{n,l}(r) = C\, e^{-\rho/2} \cdot \rho^{l}\, L_{n+l}^{2l+1}(\rho)$$

$$C = -\left[\frac{\alpha^3 (n-l-1)!}{2n\{(n+l)!\}^3}\right]^{1/2}$$

Where,

$$\alpha = \frac{2z}{na_0} \quad \text{and}$$

$$\rho = \frac{2zr}{na_0}$$

$$C = -\left[\frac{\alpha^3 \cdot 0!}{2\times 1^3}\right]^{1/2}$$

$$= -\left[\frac{\left(\frac{2}{a_0}\right)^3}{2}\right]^{1/2}$$

$$= -\left(\frac{4}{a_0^3}\right)^{1/2}$$

$$L_{n+l}^{2l+1}(\rho) = L_1^1(\rho)$$

$$= \frac{d^s}{d\rho^s}\left[e^{\rho}\cdot\frac{d^r}{d\rho^r}\left(\rho^r \cdot e^{-\rho}\right)\right]$$

$$= \frac{d}{d\rho}\left[e^{\rho}\cdot\frac{d}{d\rho}\left(\rho\cdot e^{-\rho}\right)\right]$$

$$= \frac{d}{d\rho}\left[e^{\rho}\left(e^{-\rho}\,1 - \rho e^{-\rho}\right)\right]$$

$$= \frac{d}{d\rho}(1-\rho)$$

$$= 0 - 1$$

$$= -1$$

$$\therefore R_{n,l}(r) = R_{1,0}(r)$$

$$= -\left(\frac{4}{a_0^3}\right)^{1/2} \cdot e^{-\rho/2} \cdot \rho^0 \cdot (-1)$$

$$= +\left(\frac{4}{a_0^3}\right)^{1/2} \cdot e^{-\rho/2}$$

$$= +\left(\frac{4}{a_0^3}\right)^{1/2} \cdot e^{-r/a_0} \qquad \boxed{\rho = \frac{2Zr}{na_0}}$$

$$= 2\,a_0^{-3/2} \cdot e^{-r/a_0}$$

Probability density $= \left\{R_{n,l}(r)\right\}^2$

$$= \left\{R_{1,0}(r)\right\}^2$$

$$= \left(2\,a_0^{-3/2} \cdot e^{-r/a_0}\right)^2$$

$$= 4\,a_0^{-3} \cdot e^{-2r/a_0}$$

Probability of finding the electron,-

$$= \int_0^{\infty} R^2(r)\, r^2\, dr$$

$$= \int_0^{\infty} 4a_0^{-3} \cdot e^{-2r/a_0}\, r^2\, dr.$$

$$= 4a_0^{-3} \cdot \frac{2!}{(2/a_0)^3}$$

$$= \frac{\cancel{4}}{\cancel{a_0^3}} \times \frac{2}{\frac{\cancel{8}\,2}{\cancel{a_0^3}}} = 1$$

$$= 1$$

i.e the wave function is normalised or, i.e there is 100% probability of finding the electron to lie in the atom.

Que: → Calculate radial wave function, Probability density and probability of finding the electron in the H-atom for 2p-orbital. or To show that the wave function is normalised.

Sol^n :→ For 2p-orbital.

$$n = 2$$
$$l = 1$$
$$\therefore \quad s = 2l+1 = 2\times1+1 = 3$$
$$r = n+l = 2+1 = 3$$
$$n-l-1 = 2-1-1 = 0$$

$$R_{n,l,}(r) = R_{2,1,}(r).$$
$$= C e^{-\rho/2} \cdot \rho^{l} \cdot L_{n+l}^{2l+1}(\rho)$$

Where

$$C = -\left[\frac{\alpha^3 (n-l-1)!}{2\{(n+l)!\}^3}\right]^{1/2}$$

$$= -\left[\frac{\alpha^3 \times 0!}{2\times(3!)^2}\right]^{1/2}$$

$$= -\left[\frac{\left(\frac{1}{a_0^3}\right)\times 1}{2\times6\times6\times6}\right]^{1/2}$$

$$\left[\alpha = \frac{2Z}{na_0} \quad n= \quad Z=2 \quad = \frac{\cancel{2}\times1}{\cancel{2}\times a_0}\right.$$

$$= -\frac{1}{12}\left(\frac{1}{6a_0^3}\right)^{1/2}$$

$$= -\frac{1}{12}\left(\frac{1}{6a_0^3}\right)^{1/2}$$

$$C = -\frac{1}{12}\left(\frac{1}{6a_0^3}\right)^{1/2}$$

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$$L_{n+l}^{2s+1}(\rho) = L_r^s(\rho)$$

$$= \frac{d^s}{d\rho^s}\left[e^{\rho}\cdot\frac{d^r}{d\rho^r}\left(\rho^r\cdot e^{-\rho}\right)\right]$$

$$= \frac{d^3}{d\rho^3}\left[e^{\rho}\cdot\frac{d^3}{d\rho^3}\left(\rho^3\cdot e^{-\rho}\right)\right]$$

$$= \frac{d^3}{d\rho^3}\left[e^{\rho}\cdot\frac{d^2}{d\rho^2}\left(3\rho^2\cdot e^{-\rho} - \rho^3 e^{-\rho}\right)\right]$$

$$= \frac{d^3}{d\rho^3}\left[e^{\rho}\cdot\frac{d}{d\rho}\left(6\rho\cdot e^{-\rho} - 3\rho^2\cdot e^{-\rho} - 3\rho^2 e^{-\rho} + \rho^3 e^{-\rho}\right)\right]$$

$$= \frac{d^3}{d\rho^3}\left[e^{\rho}\cdot\left(6\cdot e^{-\rho} - 6\rho e^{-\rho} - 6\rho\cdot e^{-\rho} + 3\rho^2 e^{-\rho} - 6\rho e^{-\rho} + 3\rho^2 e^{-\rho}\right) + 3\rho^2 e^{-\rho} - \rho^3 e^{-\rho}\right]$$

$$= \frac{d^3}{d\rho^3}\left(6 - 6\rho - 6\rho + 3\rho^2 - 6\rho + 3\rho^2 + 3\rho^2 - \rho^3\right)$$

$$= \frac{d^2}{d\rho^2}\left(0 - 6 - 6 + 6\rho - 6 + 6\rho + 6\rho - 3\rho^2\right)$$

$$= \frac{d}{d\rho}\left(-0 - 0 + 6 - 0 + 6 + 6 - 6\rho\right)$$

$$= 0 - 0 + 0 + 0 - 6$$

$$= -6$$

$$\therefore R_{n,l}(r) = R_{2,1}(r) = C e^{-\rho/2}\cdot\rho^l\, L^{2l+1}(\rho)$$

$$= -\frac{1}{12}\left(\frac{1}{6a_0^3}\right)^{1/2}\cdot e^{-\rho/2}\cdot\rho^1\cdot$$

$$= +\frac{1}{\cancel{12}\cdot 2}\left(\frac{1}{6a_0^3}\right)^{1/2}\cdot e^{-r/2a_0}\cdot\frac{r}{a_0}$$

$$\boxed{\rho = \frac{2Zr}{na_0} = \frac{\cancel{2}\cdot 1\cdot r}{\cancel{2}a_0}}$$

$$= \frac{1}{2}\left(\frac{1}{6a_0^3}\right)^{1/2}\cdot\frac{r}{a_0}\cdot e^{-r/2a_0}$$

$$= \frac{1}{2}\left(\frac{1}{6a_0^5}\right)^{1/2}\cdot r\cdot e^{-r/2a_0}$$

$$R_{2,1}(r) = \frac{1}{2}\left(\frac{1}{6a_0^5}\right)^{1/2} \cdot r \cdot e^{-r/2a_0}$$

Probability density :→

$$\left\{R_{2,1}(r)\right\}^2 = \left\{\frac{1}{2}\left(\frac{1}{6a_0^5}\right)^{1/2} \cdot r \cdot e^{-r/2a_0}\right\}^2$$

$$= \frac{1}{4} \cdot \frac{1}{6a_0^5} \cdot r^2 \cdot e^{-r/a_0}$$

Normalisation :—

$$\int_0^\infty \frac{1}{24a_0^5} \cdot r^2 \cdot e^{-r/a_0} \cdot r^2 \, dr$$

$$= \int_0^\infty \frac{1}{24a_0^5} r^4 \cdot e^{-r/a_0} \, dr$$

$$= \frac{1}{24a_0^5} \int_0^\infty r^4 \cdot e^{-r/a_0} \, dr$$

$$= \frac{1}{24a_0^5} \times \frac{4!}{\left(\frac{1}{a_0}\right)^{4+1}}$$

$$= \frac{1}{\cancel{24a_0^5}} \times \frac{\cancel{4 \times 3 \times 2}}{\frac{1}{a_0^5}} = 1$$

$$= 1$$

i.e the wavefunction is normalised

or i.e there is 100% probability of findin the electron to lies inside the atom.