Que. :→ Determine the radial part of the wave function for 2p-orbital of the H-atom and find the probability of finding the electron between $r=0$ and $r=\infty$. (or show that the wavefunction is normalised).

Sol^n. → For 2p-orbital,

$$n = 2$$
$$l = 1$$
$$S = 2l+1 = 3$$
$$r = n+l = 3$$

∴ Associate Laguerre polynomial is given by,

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

or, $$L_3^3\,\rho = \frac{d^3}{d^3\rho}\left[e^{\rho}\cdot\frac{d^3}{d^3\rho}\left(\rho^3\cdot e^{-\rho}\right)\right]$$

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

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

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

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

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

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

$$= -6$$

$$R(r) = -\left[\left(\frac{2Z}{na_0}\right)^3 \frac{(n-l-1)!}{2n\{(n+l)!\}^3}\right]^{1/2} e^{-\rho/2} \cdot \rho^l \times L_{n+l}^{2l+1}(\rho)$$

$\boxed{(n=2) \text{ and } l=1}$

$$= -\left[\left(\frac{1}{a_0}\right)^3 \frac{1}{4 \times 6 \times \cancel{6} \times \cancel{6}}\right]^{1/2} e^{-\rho/2} \cdot \rho^1 \times (-\underline{6})$$

$$= +\left[\frac{1}{a_0^3} \cdot \frac{1}{24}\right]^{1/2} e^{-\rho/2} \rho$$

$$\boxed{\rho = \frac{2Zr}{na_0}}$$

$$= \frac{1}{2\sqrt{6}} \left(\frac{1}{a_0}\right)^{3/2} e^{-\frac{2r}{2a_0}} \cdot (\cancel{\rho}) \times \frac{\cancel{2}Zr}{\cancel{n}a_0}$$

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

$$R^2(r) = \frac{1}{4 \times 6} \cdot \frac{1}{a_0^3} \cdot \left(\frac{r^2}{a_0^2}\right) e^{-r/a_0}$$

$$= \frac{r^2 e^{-r/a_0}}{24 a_0^5}$$

- Determine the probability of finding the electron in the atom.

$$\int_0^\infty R(r) \cdot R^*(r) \cdot r^2 \, dr$$

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

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

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

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

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

i.e. there is 100 % probability.

Legendre Polynomial

$$P_l(x) = \frac{1}{2^l \times l!} \cdot \frac{d^l}{dx^l}(1-x^2)^l$$

Leg. poly. of degree l.

Associated Legendre Polynomial

$$P_l^m(x) = (1-x^2)^{|m|/2} \frac{d^{|m|}}{dx^{|m|}} \cdot P_l(x)$$

Thus

for s-orbital,

$l = 0, \quad m = 0$

$$P_0^0(x) = P_0(x) = 1$$

For p_z-orbital. $\quad l = 1, \; m = 0$

$$P_1^0(x) = P_1(x)$$

$$= \frac{1}{2^1 \times 1!} \cdot \frac{d}{dx}(1-x^2)^1$$

$$= \frac{1}{2}(-2x)$$

Laguerre Polynomial :→

$L_n(x)$ = Lag. Poly. of n^{th} degree in x,

$$= e^{x} \cdot \frac{d^n}{dx^n}\left(x^n e^{-x}\right)$$

Associated Laguerre Polynomial —

$L_n^m(x)$ = Assoc. Lag. Polynomial in x of degree $n-m$.

$$= (-1)^n \cdot \frac{n!}{(n-m)!}\left[x^{n-m} - \frac{n(n-m)}{1!} x^{n-m-1} + \frac{n(n-1)(n-m)(n-m-1)}{2!} \cdot x^{n-m-2} + \cdots\cdots\cdots\right]$$

$L_{n+l}^{2l+1} \longrightarrow$ is ass. Lag. poly. of degree $n-l-1$.

29

Hermite Polynomial:

$$H_n(x) = (-1)^n e^{x^2} \cdot \frac{d^n}{dx^n}\left(e^{-x^2}\right)$$

↘ Hermite polynomial of degree n in (x)

$$H_0(x) = (-1)^0 \cdot e^{x^2} \cdot \frac{d^0}{dx^0} \cdot \left(e^{-x^2}\right)$$

$$= e^{x^2} \cdot e^{-x^2} = e^0 = 1$$

$$H_1(x) = (-1)^1 e^{x^2} \cdot \frac{d}{dx}\left(e^{-x^2}\right)$$

$$= -1 \cdot e^{x^2} e^{-x^2}(-2x)$$

$$= +2x.$$

$$H_2(x) = (-1)^2 e^{x^2} \cdot \frac{d^2}{dx^2}\left(e^{-x^2}\right)$$

$$= -e^{x^2} \cdot \frac{d}{dx}\left(-2x \cdot e^{-x^2}\right)$$

$$= -e^{x^2}\left(-2x \times -2x\, e^{-x^2} + 2\, e^{-x^2}\right)$$

$$= +4x^2 - 2$$

Recursive formula for Hermite Polynomial.

$$\xi H_n(\xi) = \frac{1}{2} H_{n+1}(\xi) + n H_{n-1}(\xi);$$