Radial wave function:-

\# for S-orbital $\Rightarrow \begin{cases} R(r) = +ve & \text{at } r=0 \\ R(r) = 0 & \text{at } r=\infty \end{cases}$

\# for other orbitals $\Rightarrow \begin{cases} R(r) = 0 & \text{at } r=0 \\ R(r) = 0 & \text{at } r=\infty \end{cases}$

General form :

$R_{n\ell}(r) = K \cdot e^{-\sigma/2} \cdot \sigma^{\ell}$ **(Polynomial of order n – ℓ – 1)**

where $\sigma = \dfrac{2Zr}{na_0}$ $\qquad a_0 = I^{st}$ Bohr's radius = 0.529Å

\#

1s $\quad (n = 1, \ell = 0)$: $\quad R_{1s}(r) = 2 \cdot \left(\dfrac{Z}{a_0}\right)^{3/2} \cdot e^{-\sigma/2}$

$\sigma^{l} = 1 \Rightarrow l = 0$
$n-l-1 = 0$
$n = 1$
1(s)

where $\sigma = \dfrac{2Zr}{na_0}$ $\qquad a_0 = I^{st}$ Bohr's radius = 0.529Å

2s $\quad (n = 2, \ell = 0)$: $\quad R_{2s}(r) = \dfrac{1}{2\sqrt{2}} \cdot \left(\dfrac{Z}{a_0}\right)^{3/2} \cdot (2 - \sigma)e^{-\sigma/2}$

$\sigma^{l} = 1 \Rightarrow l = 0$
$n-l-1 = 1$
$n = 2 \Rightarrow 2(s)$

2p $\quad (n = 2, \ell = 1)$: $\quad R_{2p}(r) = \dfrac{1}{2\sqrt{6}} \cdot \left(\dfrac{Z}{a_0}\right)^{3/2} \cdot \sigma \cdot e^{-\sigma/2}$

$\sigma^{l} = \sigma \Rightarrow l = 1$
$n-l-1 = 0 \Rightarrow n = 2 \Rightarrow$ 2p

3s $\quad (n = 3, \ell = 0)$: $\quad R_{3s}(r) = \dfrac{1}{9\sqrt{3}} \cdot \left(\dfrac{Z}{a_0}\right)^{3/2} \cdot (6 - 6\sigma + \sigma^2)e^{-\sigma/2}$

$\sigma^{l} = 1 \Rightarrow l = 0$
$n-l-1 = 2$
$n = 3 \Rightarrow 3(s)$

3p $\quad (n = 3, \ell = 1)$: $\quad R_{3p}(r) = \dfrac{1}{9\sqrt{6}} \cdot \left(\dfrac{Z}{a_0}\right)^{3/2} \cdot \sigma(4 - \sigma)e^{-\sigma/2}$

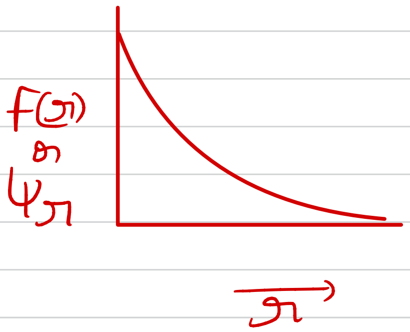
$\sigma^{l} = \sigma \Rightarrow l = 1$
$n-l-1 = 1 \Rightarrow n = 3$
3p

3d $\quad (n = 3, \ell = 2)$: $\quad R_{3d}(r) = \dfrac{1}{9\sqrt{30}} \cdot \left(\dfrac{Z}{a_0}\right)^{3/2} \cdot \sigma^2 \cdot e^{-\sigma/2}$

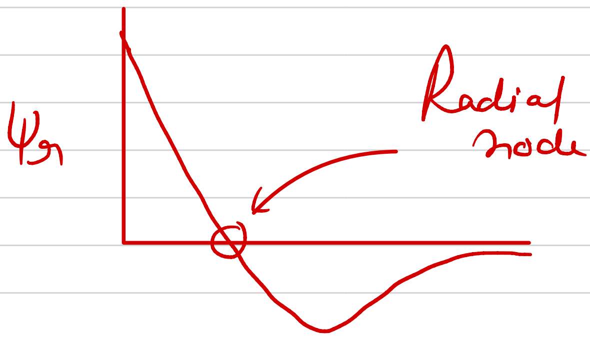
$\sigma^{2} = \sigma^{l} \Rightarrow l = 2$
$n-l-1 = 0 \Rightarrow n = 3$
3d

Graph R(r) vs r:-

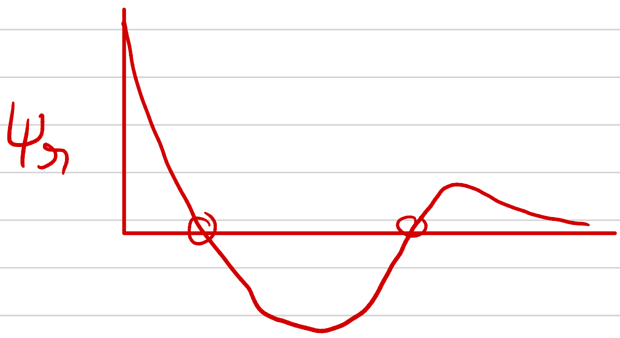
1. 1(s) $n-l-1=0$



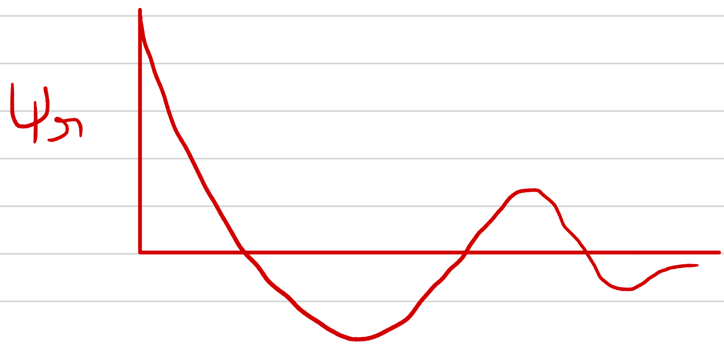
2. 2(s) $n-l-1=1$



3. 3(s) $n-l-1=2$

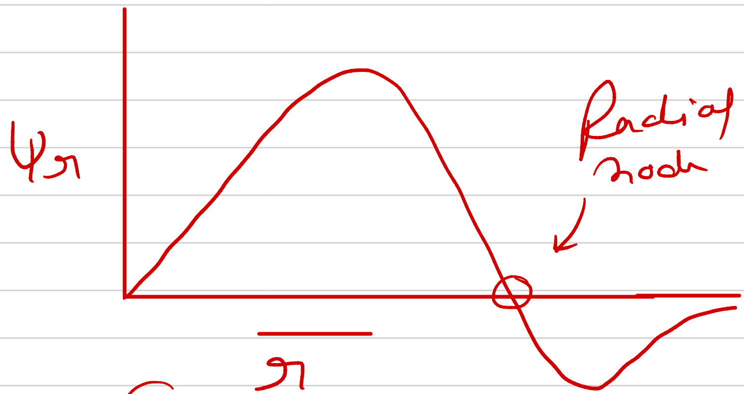


4. 4(s) $n-l-1=3$

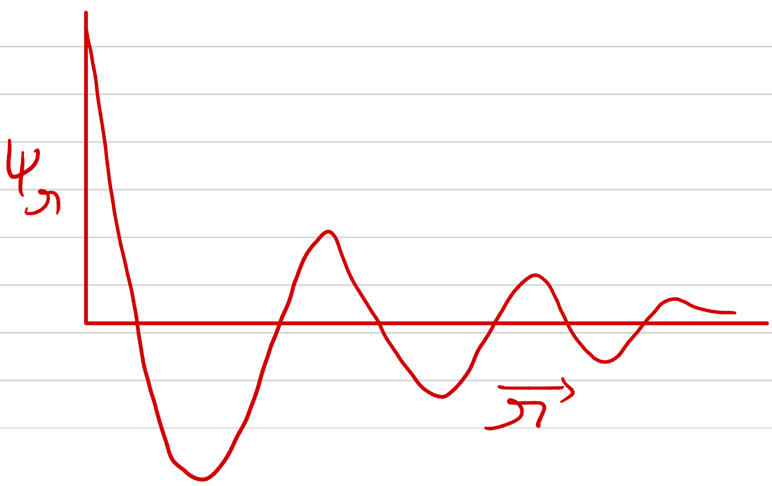


5. 2(P) $n-l-1=0$

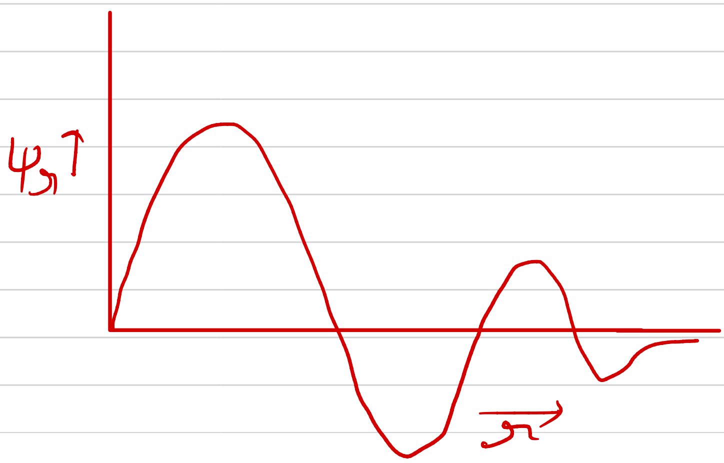
6. 3(P) $n-l-1=1$



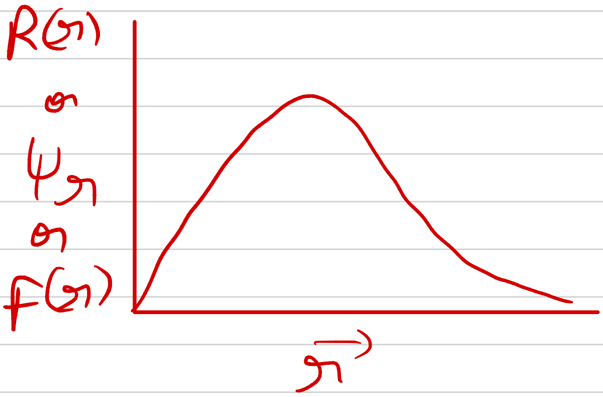
7. 7(S) $n-l-1=6$



8. 5(P) $n-l-1=3$



(9) 3(d) $n-l-1 = 0$



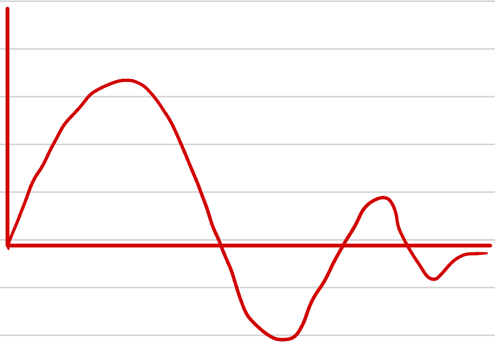
(10) 4(d) $n-l-1 = 1$

$2p \equiv 3d \equiv 4f$

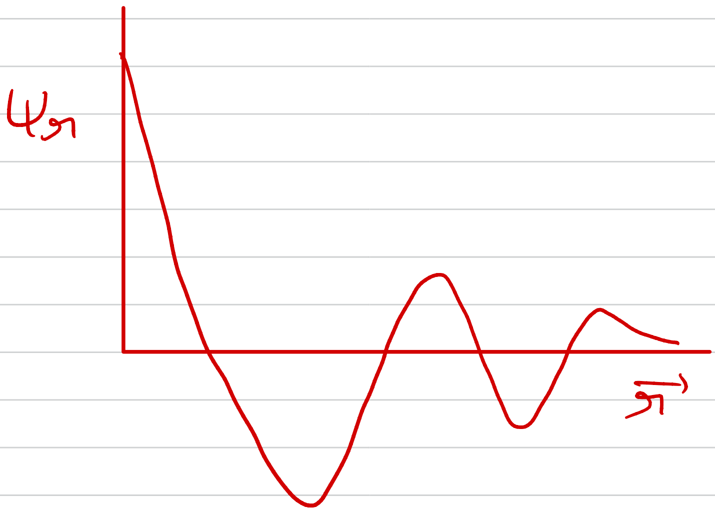
$3p \equiv 4d \equiv 5f$

eg:

(1) 5p $n-l-1 = 3$

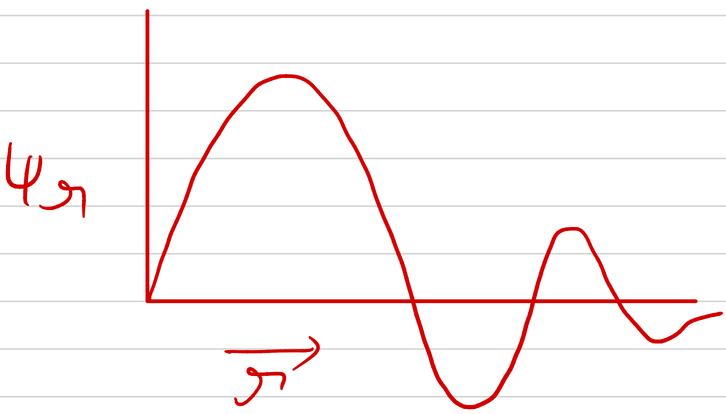


(2) 5(s) $n-l-1 = 4$

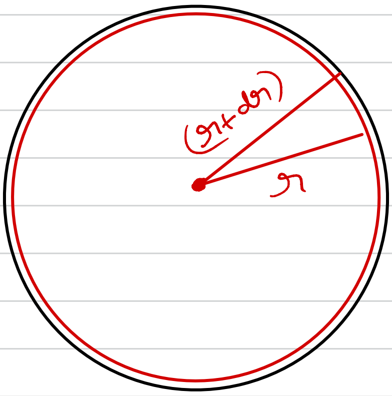


(3) 6(d)

$n-l-1 = 3$



Radial probability distribution function:-



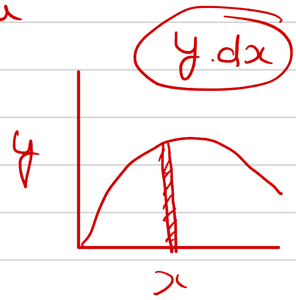
\# $dV = 4\pi r^2 . dr$

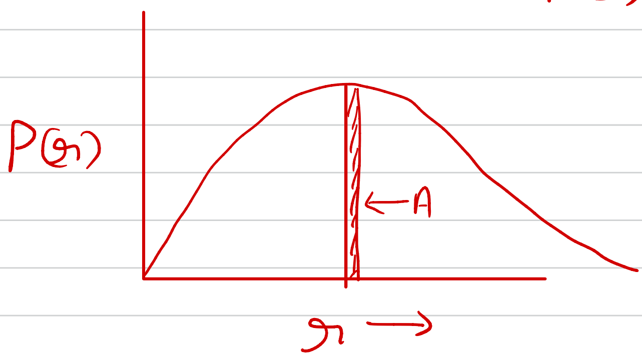
$[R(r)]^2$ = Radial probability density

= Probability of finding e^- at a distance r from the nucleus.

Radial Probability of e^- at a distance r from the nucleus $= [R(r)]^2 \times dV$

$$= \underbrace{4\pi r^2 [R(r)]^2}_{P(r)} . dr$$



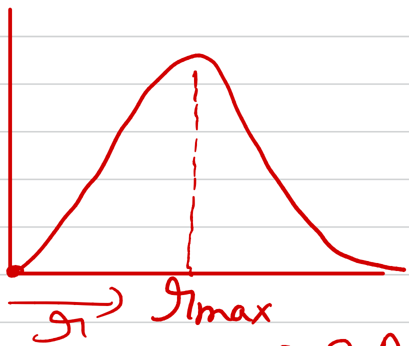


$P(r).dr = A$

$P(r)$ Vs r

① 1(s) $n-l-1=0$

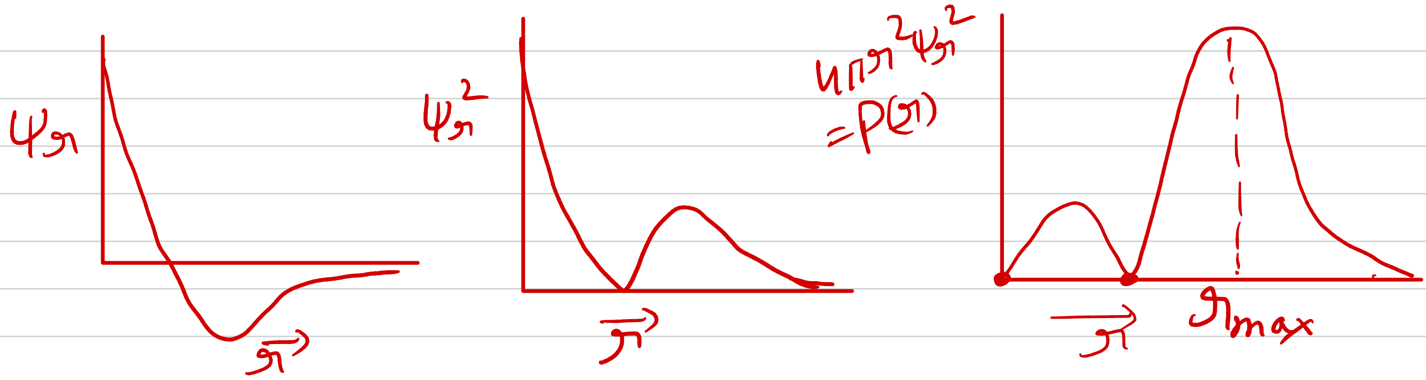
$4\pi r^2 \psi_r^2 = P(r)$



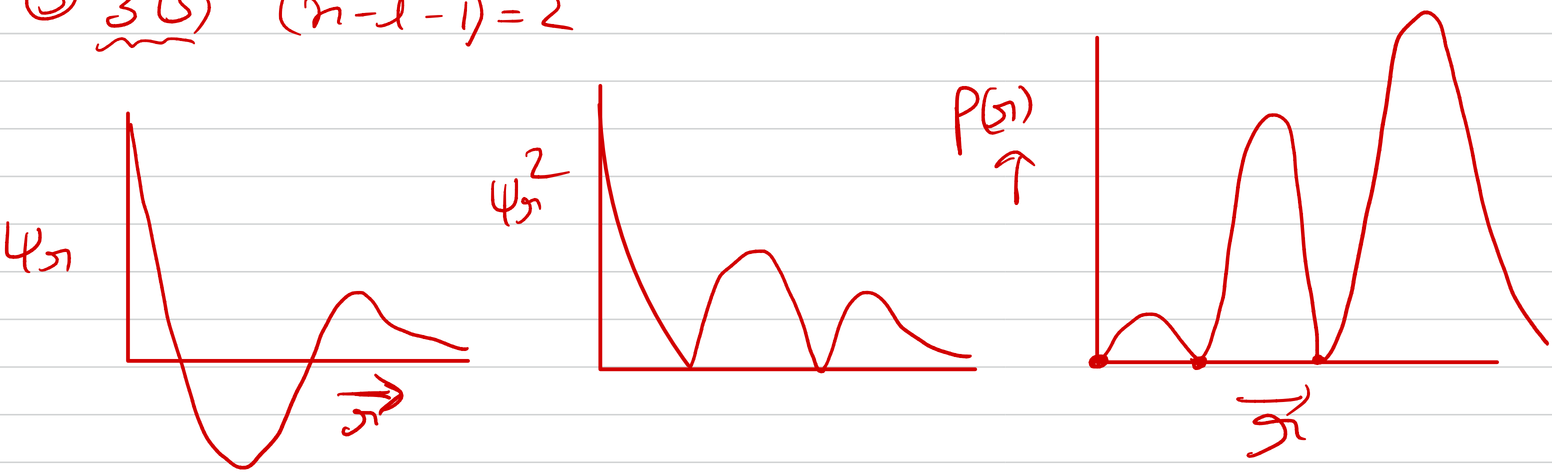
$r_{max} = 0.529\ A^\circ$

For 1(s) in H atom

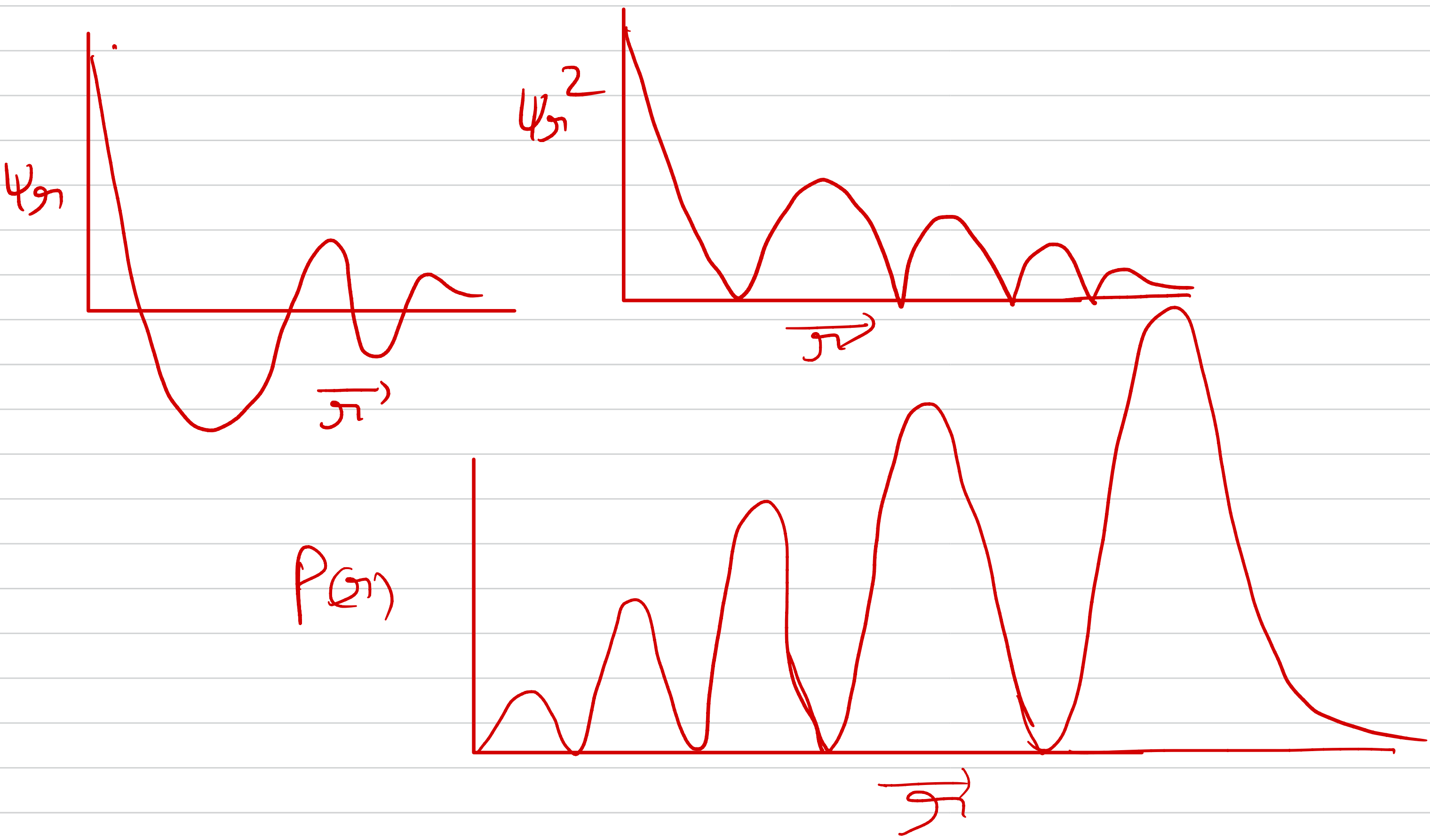
② 2(S) $(n-l-1)=1$



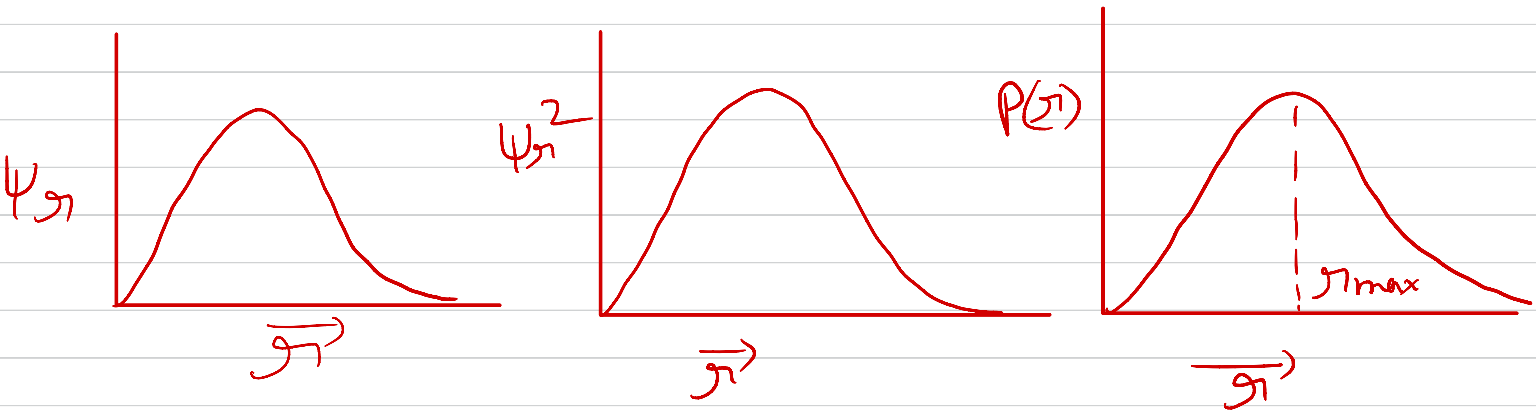
③ 3(S) $(n-l-1)=2$



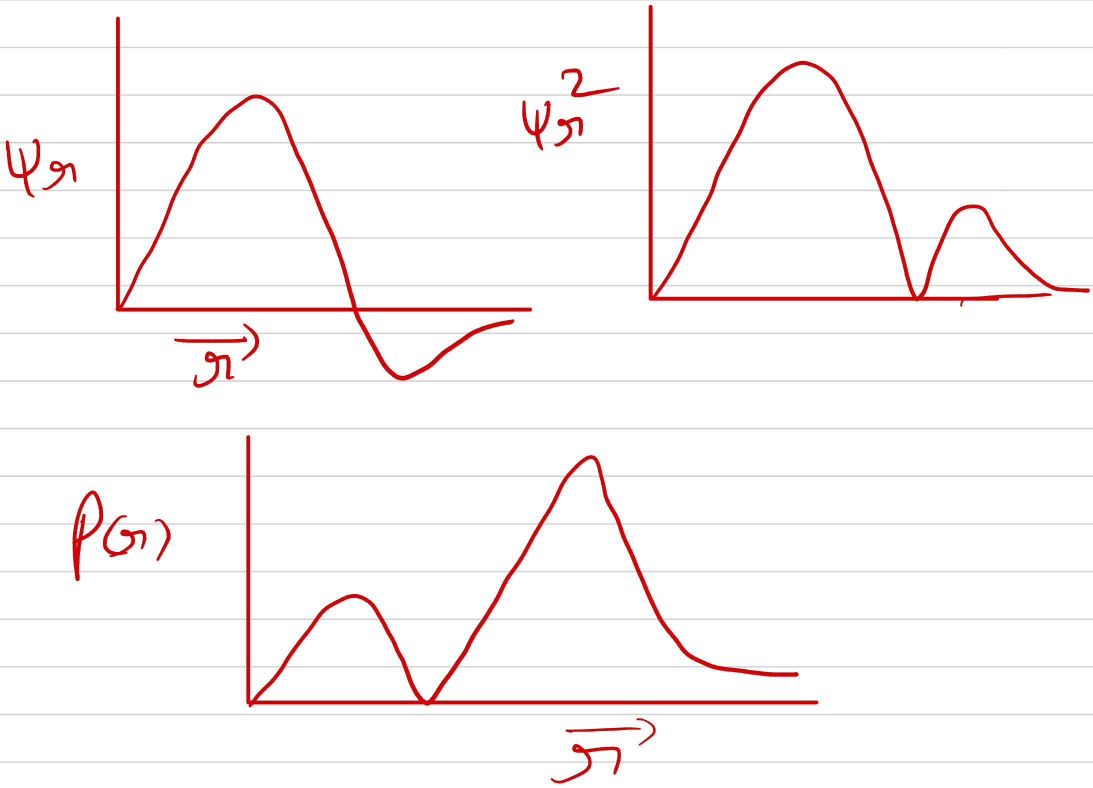
④ 5(S) $(n-l-1)=4$



⑤ $2(P)$ $n-l-1=0$



⑥ $3(P)$ $(n-l-1)=1$



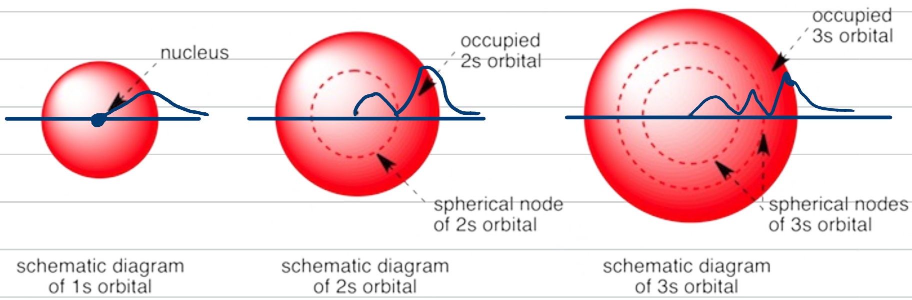
Angular function:- $Y(\theta,\phi)_{l,m}$

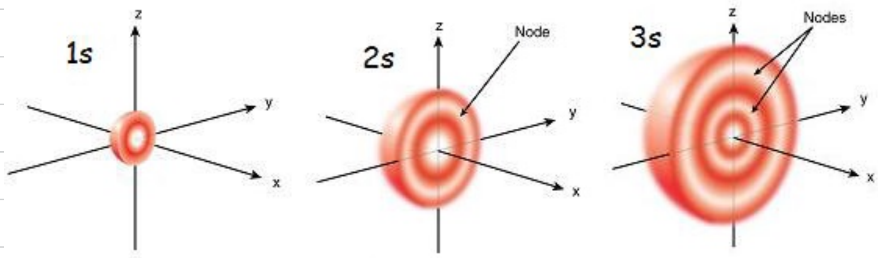
No of angular nodes = l

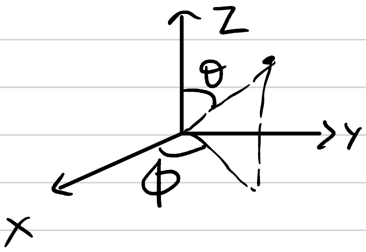
at angular node $Y(\theta,\phi) = 0$

① S orbital:-

$\ell = 0, m = 0$, $Y(\theta,\phi) = \Theta(\theta) \cdot \Phi(\phi) = \sqrt{\frac{1}{4\pi}}$ = Constant





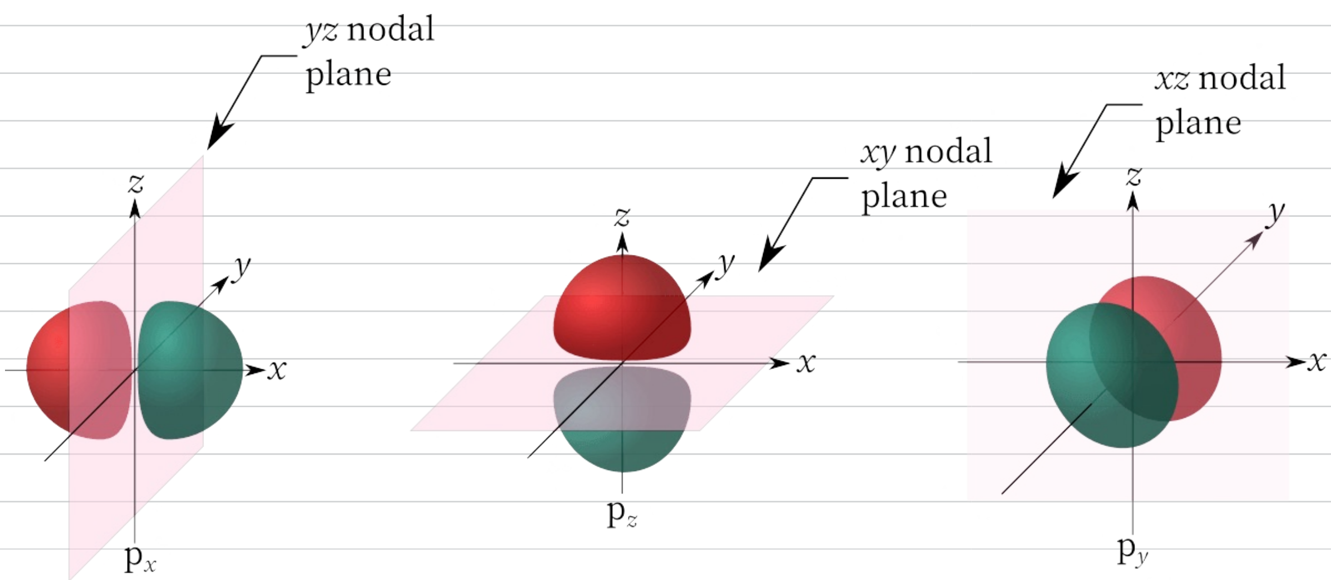


② P orbital:-

p_x-orbital : $\ell = 1, m = \pm 1$ $\quad \Theta(\theta) \cdot \Phi(\phi) = \sqrt{\frac{3}{4\pi}} \cdot \sin\theta\cos\phi$ ⇒ $\theta = 0, \phi = \frac{\pi}{2}$ ⇒ YZ

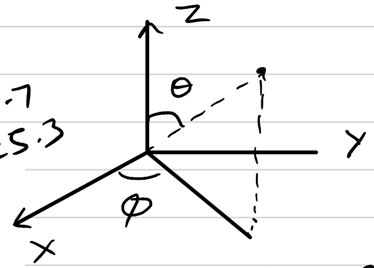
p_y-orbital : $\ell = 1, m = \mp 1$ $\quad \boxed{\Theta(\theta) \cdot \Phi(\phi) = \sqrt{\frac{3}{4\pi}} \cdot \sin\theta\cancel{\cos\phi}}$ $\sin\phi$ ⇒ $\theta = 0, \phi = 0$ ⇒ XZ

p_z-orbital : $\ell = 1, m = 0$ $\quad \Theta(\theta) \cdot \Phi(\phi) = \sqrt{\frac{3}{4\pi}} \cdot \cos\theta$ ⇒ $\theta = \frac{\pi}{2}$ ⇒ XY



③ d orbital:- No of angular node = l = 2

$\theta = 54.7$
$\theta = 125.3$



d_{z^2} -orbital : $\ell = 2,\ m = 0$ $\quad \Theta(\theta)\ .\ \Phi(\phi) = \sqrt{\frac{5}{16\pi}}(3\cos^2\theta - 1)$

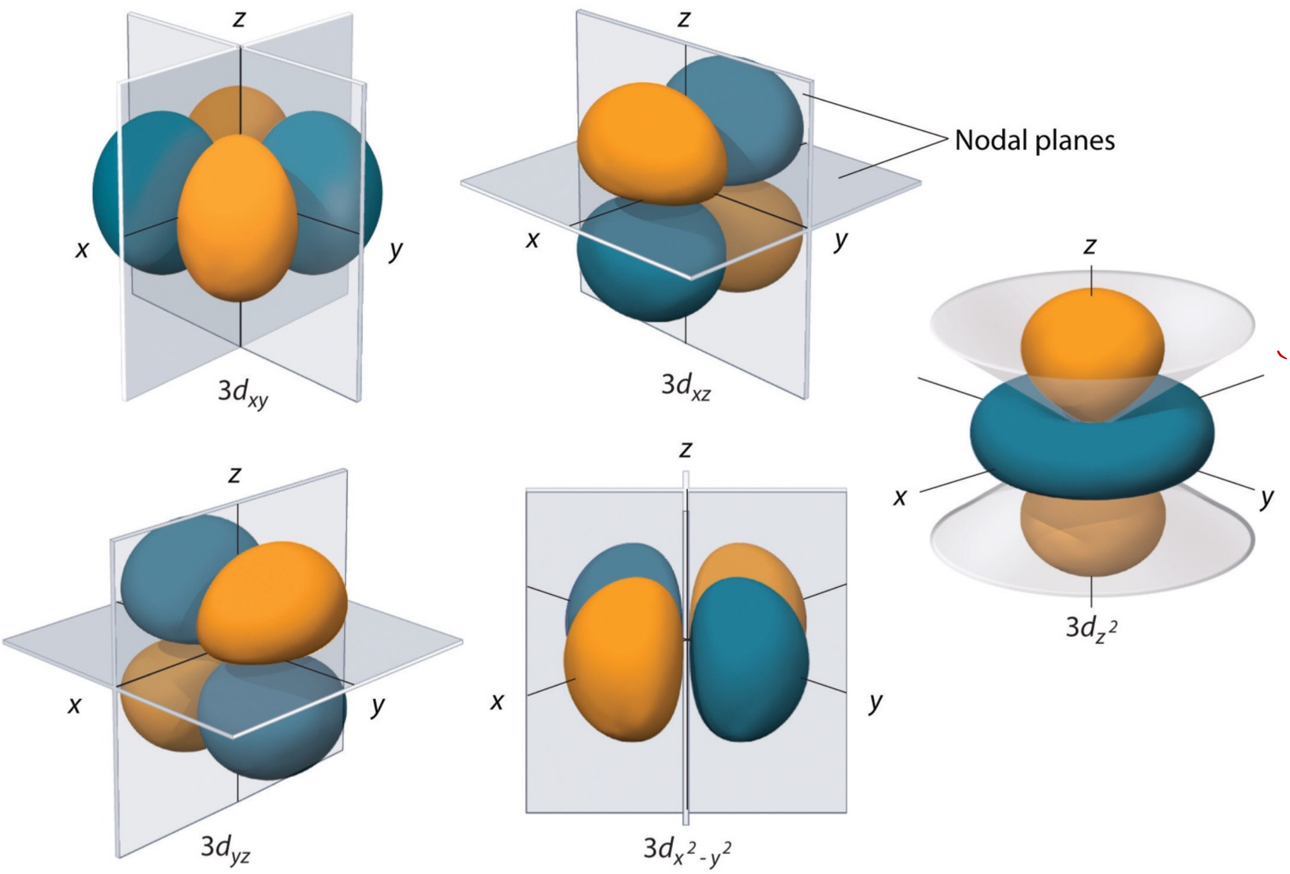
$d_{x^2-y^2}$ -orbital : $\ell = 2,\ m = -2$ $\quad \Theta(\theta)\ .\ \Phi(\phi) = \sqrt{\frac{15}{4\pi}} \cdot \sin^2\theta \cos 2\phi$ $\Rightarrow \left(\theta=0, \phi=\frac{\pi}{4}\right)\ \left(\theta=0, \phi=\frac{3\pi}{4}\right)$

d_{xy} -orbital : $\ell = 2,\ m = +2$ $\quad \Theta(\theta)\ .\ \Phi(\phi) = \sqrt{\frac{15}{4\pi}} \cdot \sin^2\theta \sin 2\phi$ $\Rightarrow \underset{XZ}{(\theta=0, \phi=0)}, \underset{YZ}{\left(\theta=0, \phi=\frac{\pi}{2}\right)}$

d_{xz} -orbital : $\ell = 2,\ m = +1$ $\quad \Theta(\theta)\ .\ \Phi(\phi) = \sqrt{\frac{15}{4\pi}} \cdot \sin\theta \cos\theta \sin 2\phi$

d_{yz} -orbital : $\ell = 2,\ m = +1$ $\quad \Theta(\theta)\ .\ \Phi(\phi) = \sqrt{\frac{15}{4\pi}} \cdot \sin\theta \cos\theta \cdot \sin\phi$

$\underset{XZ}{(\theta=0, \phi=0)}\ \underset{XY}{\left(\frac{\pi}{2}, 0\right)}$



$n - l = 4$

$l = 3$

$n = 7$

The radial probability distribution curve of an orbital of H has '4' local maxima. If orbital has 3 angular node then orbital will be :

(a) 7*f* (b) 8*f*

(c) 7*d* (d) 8*d*

The Schrodinger wave equation for hydrogen atom of 4*s*-orbital is given by :

$$\psi(r) = \frac{1}{16\sqrt{4}}\left(\frac{1}{a_0}\right)^{3/2}[(\sigma-1)(\sigma^2-8\sigma+12)]e^{-\sigma/2}$$

where a_0 = 1st Bohr radius and $\sigma = \frac{2r}{a_0}$. The distance from the nucleus where there will be no radial node will be :

(a) $r = \frac{a_0}{2}$ (b) $r = 3a_0$

(c) $r = a_0$ (d) $r = 2a_0$

$\psi(r) = 0$

$\sigma = 1 \quad \sigma = 2, 6 \quad = \frac{2r}{a_0}$

$r = \frac{a_0}{2}, \quad a_0, \quad 3a_0$

For an orbital, having no planar angular nodes following the equation :

$$\psi_{(r)} = Ke^{-r/K'} \cdot r^2(K'' - r)$$

Identify the orbital :

(a) $4d_{z^2}$ (b) 2*s*

(c) $3d_{z^2}$ (d) $4d_{xy}$

The Schrodinger wave equation for hydrogen atom is $\psi_{2s} = \frac{1}{4\sqrt{2\pi}}\left(\frac{1}{a_0}\right)^{3/2}\left(2-\frac{r}{a_0}\right)e^{-r/a_0}$, where a_0 is Bohr's radius. If the radial node in 2*s* be at r_0, then r_0 would be equal to :

(a) $\frac{a_0}{2}$ (b) $2a_0$

(c) $\sqrt{2}a_0$ (d) $\frac{a_0}{\sqrt{2}}$

$\psi_r = 0$

$r = 2a_0 = r_0$

Choose the **correct** statement(s).

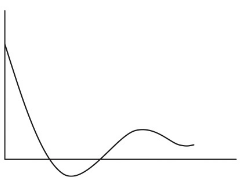
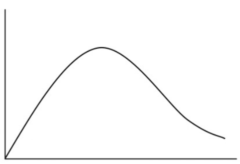
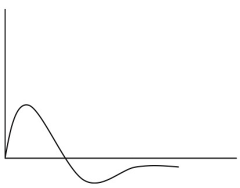
(a) The orbital wave function or ψ for an electron has no physical meaning

(b) Square of wave function (ψ^2) at a point gives the probability density of the electron at that point.

(c) Boundary surface diagrams of constant probability density for different orbitals give a fairly good representation of the shapes of the orbitals.

(d) All of the above

Match the columns.

Column I (Orbital)	**Column II (R vs. r Graph)**
(A) 3*s*	(P) 
(B) 4*s*	(Q) 
(C) 2*p*	(R) 
(D) 3*p*	(S)