CH102 — Tu 4

1 (a) $\psi(r,\theta,\phi) = N e^{-r/a_0}$

$$|\psi|^2 = N^2 e^{-2r/a_0}$$

$$\int_0^\infty |\psi|^2 dr = \int_0^\infty N^2 e^{-2r/a_0} \cdot 4\pi r^2 dr = 1$$

$$4\pi N^2 \int_0^\infty r^{2} e^{-2r/a_0} dr = 1$$

$$4\pi N^2 \quad \frac{2!}{(2/a_0)^3} = 1$$

$$\cancel{4}\pi N^2 \cdot \frac{\cancel{2}}{\cancel{8}/a_0^3} = 1$$

$$N^2 a_0^3 \pi = 1 \quad \Rightarrow \quad N = \frac{1}{a_0\sqrt{a_0\pi}}$$

(b) $r_{av} = \langle \psi | r | \psi \rangle$

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

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

$$= \frac{\cancel{4\pi a_0}}{} \quad \frac{\cancel{2\pi}}{\cancel{a_0^3}\cancel{\pi}} \times \frac{\cancel{4}\times 3\times\cancel{2}\times 1 \times \cancel{a_0^4} a_0}{\cancel{4}\times\cancel{4}}$$

$$= \underline{3a_0}$$

(2)

$$\psi_{3d_{z^2}} = N r^2 e^{-r/3} \left(3\cos^2\theta - 1\right)$$

In general

$$\psi = R(r) \cdot \Theta(\theta) \cdot \Phi(\phi)$$

where $\phi = A e^{+im\phi}$ $\rightarrow m \in \mathbb{Z}$, $|m| \leq l$

here $\boxed{\phi = 0}$ in $\boxed{\phi = 2\pi}$ $0 \leq \phi \leq 2\pi$

θ: $3\cos^2\theta = 1$

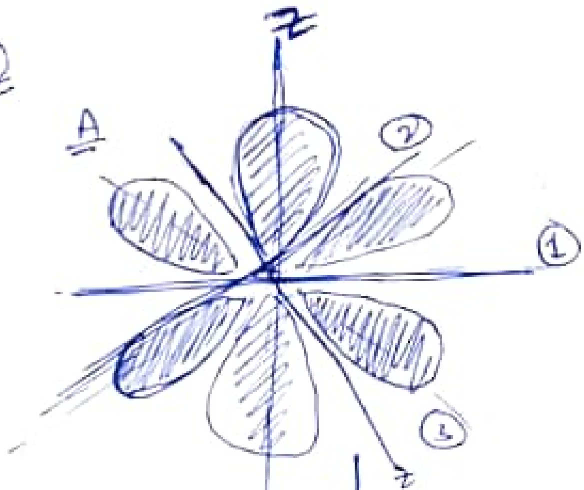
$\cos\theta = \frac{+1}{\sqrt{3}}$ or $\frac{-1}{\sqrt{3}}$

$\theta = \cos^{-1}\left(\frac{1}{\sqrt{3}}\right)$ and $\cos^{-1}\left(\frac{-1}{\sqrt{3}}\right)$

where $0 \leq \theta \leq 2\pi$

(3)

A



Angular node = (3) = l

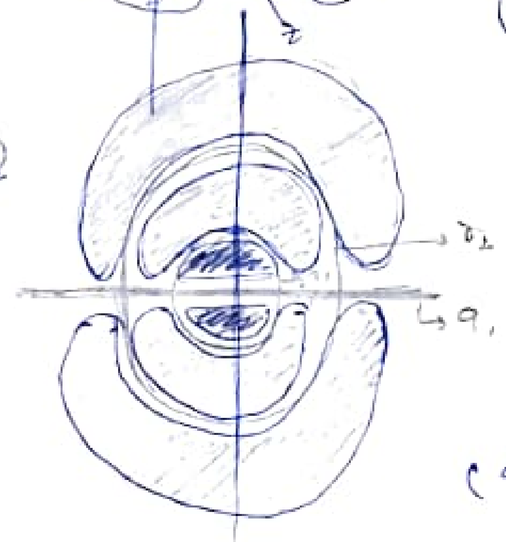
Radial Node = (0) $n-l-1$

$n = 4$

$m_l = 0$

$(4f_{z^3})$

B



Angular nodes = (1) = l

Radial nodes = (2) = $n-l-1$

$n = 4$

$m_l = 0$

$(4p_z)$

- Tu 4

(c)

Angular nodes = 4 = l

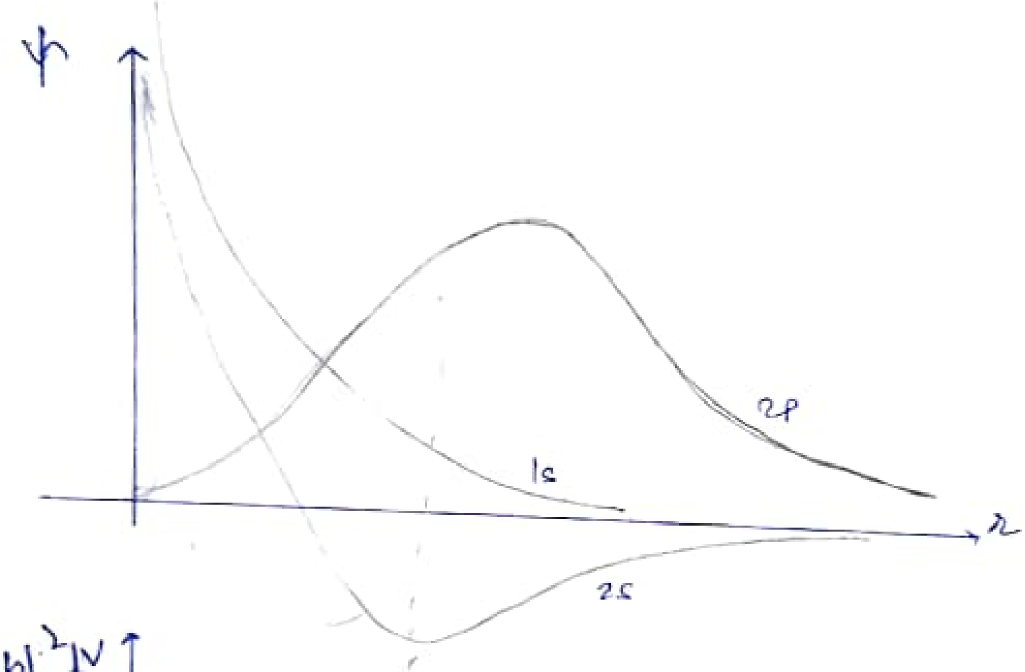
Radial node = 4 = $n-l-1$

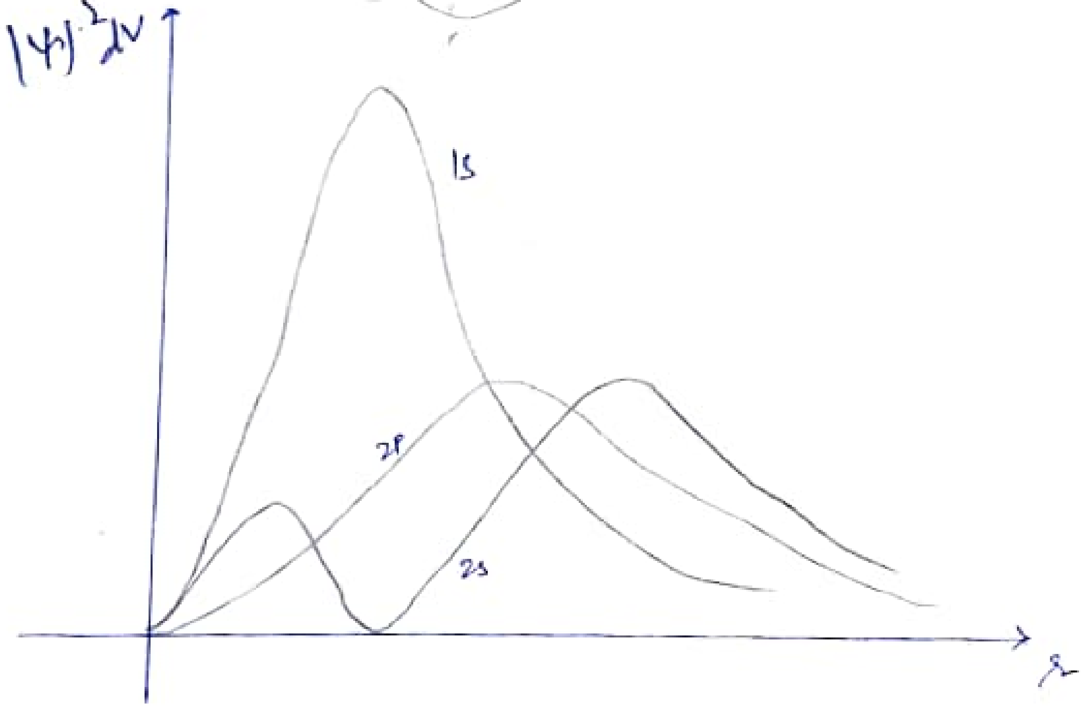
$n=9$

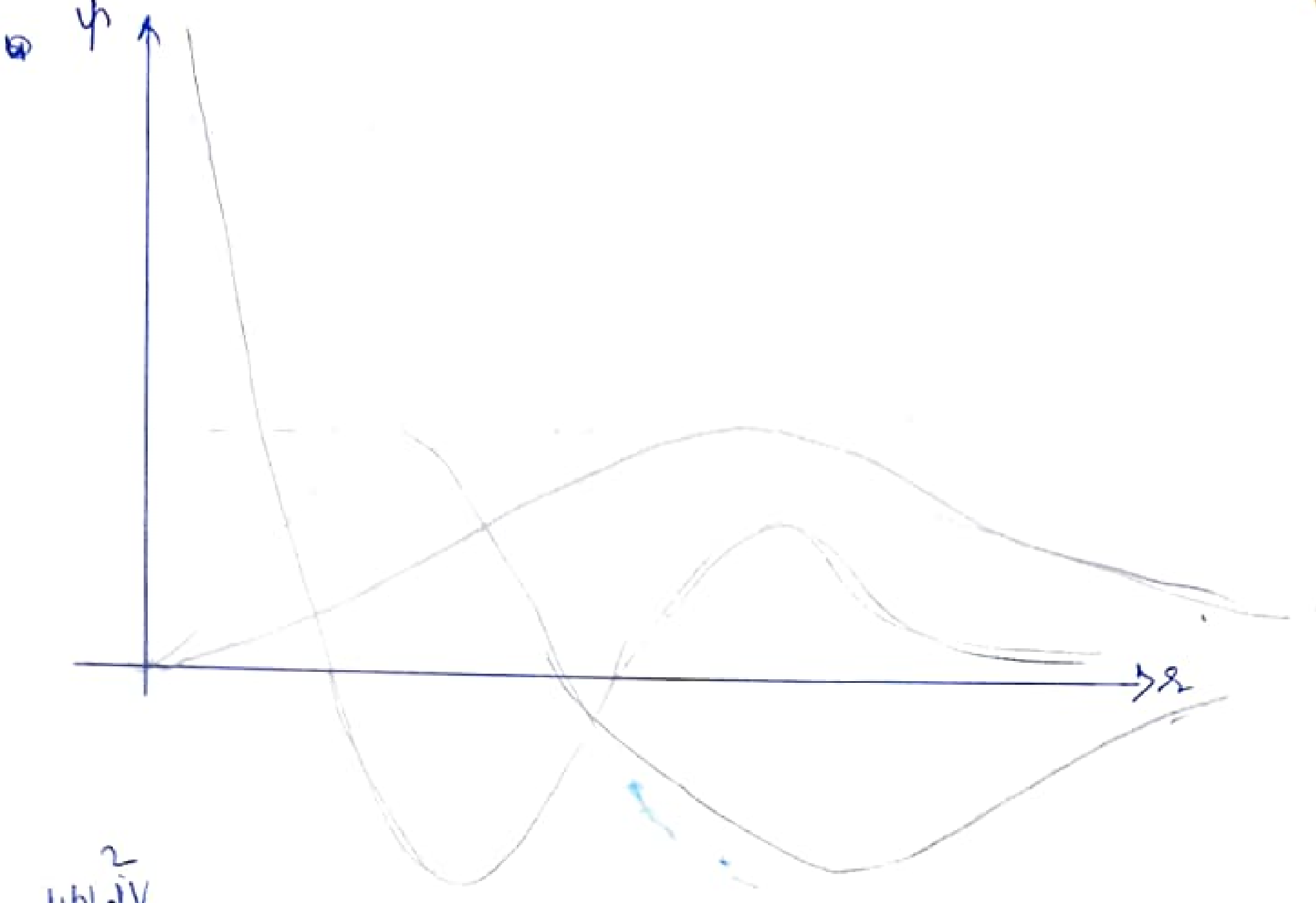
$m=0$

(5)

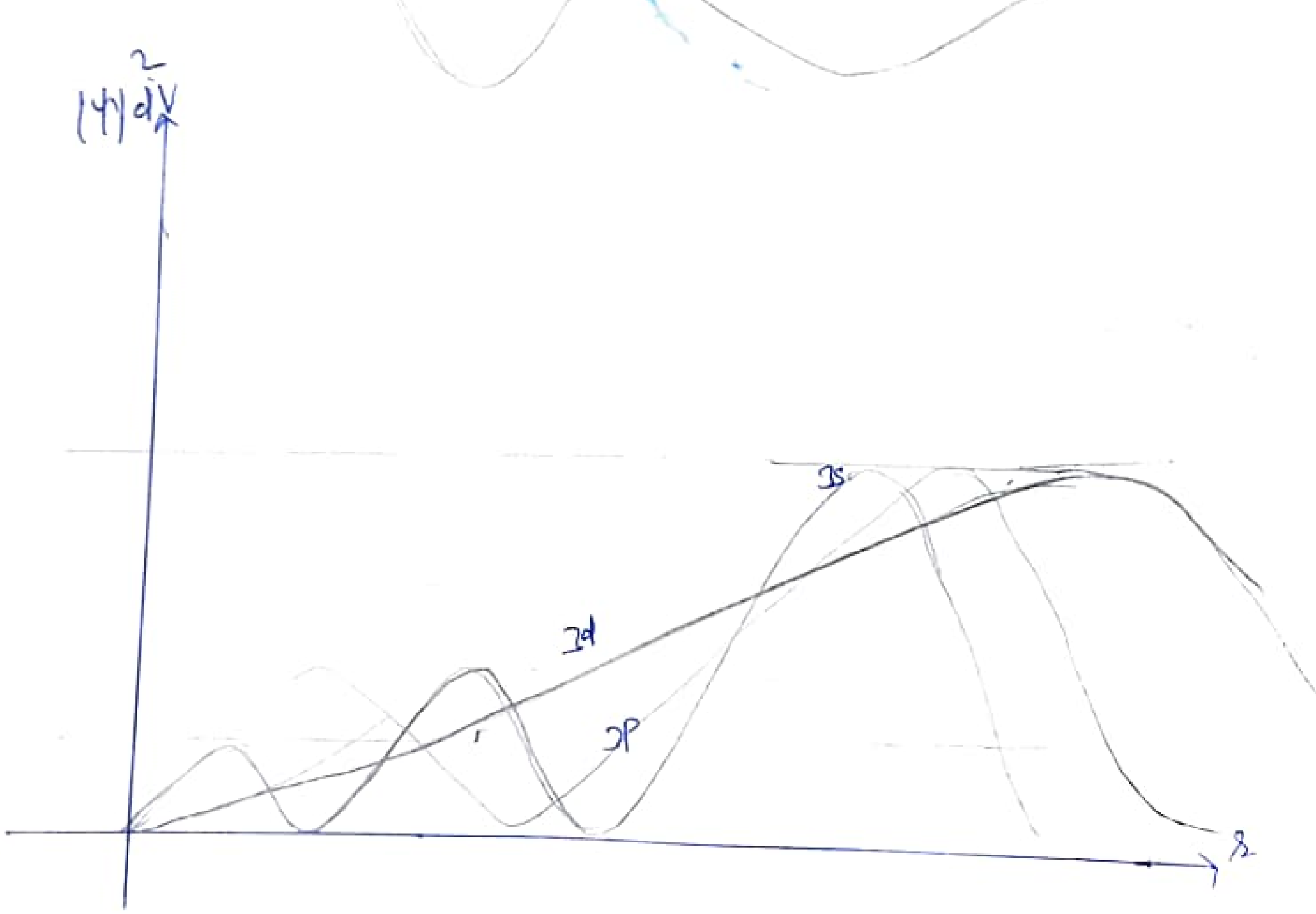
$r^l e^{-\frac{Zr}{na_0}}$







ψ
r



|ψ|²dV
3s
3d
3p
r

(1) (i) $\psi_{1s} = \frac{2}{a_0^{3/2}} e^{-r/a_0}$

$\frac{\partial \psi}{\partial r}$

$dP = |\psi|^2 4\pi r^2 dr$

$dP = \cancel{|\psi|^2} \cdot \frac{4}{a_0^3} e^{-2r} \cdot 4\pi r^2$

$\frac{dP}{dr} = \frac{d}{dr}\left[\frac{16\pi}{a_0^3} r^2 e^{-2r/a_0}\right]$

$\frac{16\pi}{a_0^3}\left[2r e^{-2r/a_0} + r^2 \cdot e^{-2r/a_0} \cdot \frac{-2}{a_0}\right]$

$= 0$

$\Rightarrow \cancel{2r} = \frac{2r^2}{a_0}$

$r = a_0$

(ii) $\psi_{2p_z} \rightarrow A r e^{-r/2a_0} \cos\theta$

$dP = A r e^{-r/2a_0} \cos\theta \cdot r^2 \sin\theta \, d\theta \, d\phi \, dr$

$\frac{\partial P}{\partial r} = 0 \Rightarrow \frac{d}{dr}(r^3 \cos\theta \, e^{-r/2a_0}) = 0$

$3r^2 e^{-r/2a_0} - \frac{r^3}{2a_0} e^{-r/2a_0} = 0$

$6a_0 = r$

$\frac{\partial P}{\partial \theta} = 0 \Rightarrow \frac{\partial}{\partial \theta}(\cos\theta\sin\theta) = 0 \quad \frac{\partial}{\partial \theta}\frac{\sin 2\theta}{2} = 0$

$\left\{\theta = (2n+1)\frac{\pi}{4}\right\} \quad \cos 2\theta = 0$