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Electronic Properties of Materials:

$$E(x,t) = E_0 e^{i(\omega t - kx)}$$

phase velocity $v_p = \frac{\omega}{k}$

The avg intensity $= \frac{1}{2} c \epsilon E_0^2$

$\downarrow$ only measurable quantity.

Born interpretation:

$\psi(x,y,z,t) \rightarrow$ function

probability to find particle $|\psi(x,y,z,t)|^2$ at x,y,z at any time t.

→ Time-independent Schrodinger Eqn:

$$\left[\frac{-\hbar^2}{2m}\nabla^2 + V\right]\psi = i\hbar\frac{\partial\psi}{\partial t}$$

$$\underbrace{\frac{-\hbar^2}{2m}\nabla^2}_{KE} + \underbrace{V}_{PE} = \text{Hamiltonian operator } (\hat{H})$$

A free particle ($V=0$) everywhere

$$\psi = A\cos\left(\frac{2\pi x}{\lambda} - \omega t\right)$$

→ oscillating everywhere.

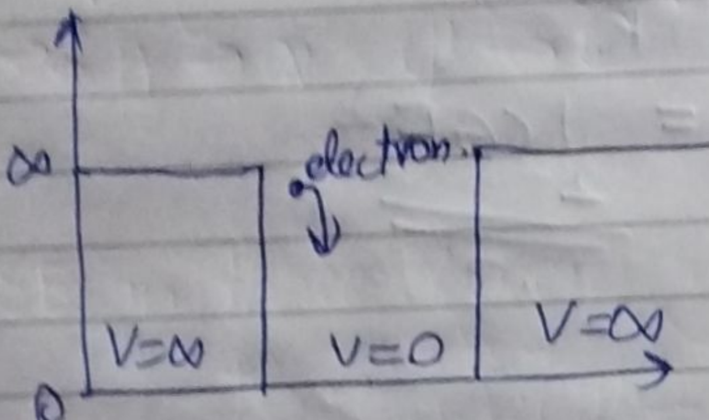
$\frac{2\pi}{\lambda} = \frac{2\pi p}{h} = k$ momentum.

$\omega = \frac{h\nu}{h} = \frac{E}{\hbar}$ → energy

$$\psi(x) = Ae^{ikx} \quad \{V=0\}$$

$$\psi^* \psi = A^2$$

Particle in a Box:



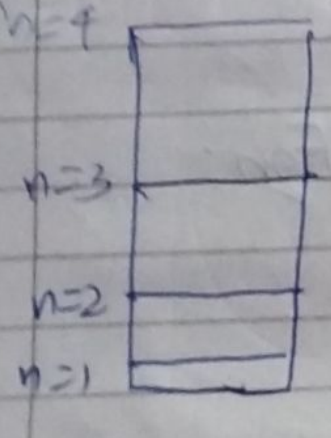
$$\psi(x) = 2Ai \sin kx$$

$$k = \frac{2\pi n}{a}$$

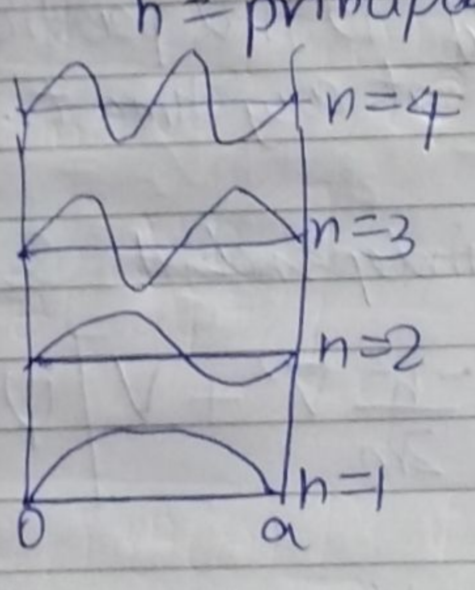
$$E = \frac{\hbar^2 k^2}{2m} = \cancel{\hbar^2 n^2} \frac{h^2 n^2}{8ma}$$

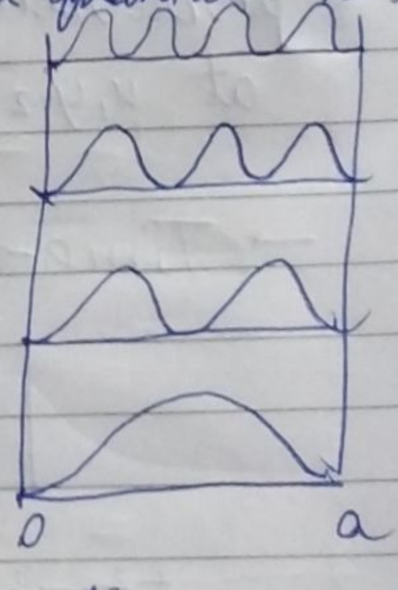
$$A = \frac{1}{\sqrt{2a}}$$

n = principal quantum no.



Energy levels in well.





→ wavefunctions are no longer continuous.

→ only discrete energy levels exist:

$n=0 \Rightarrow E=0$ → particle does not exist anywhere

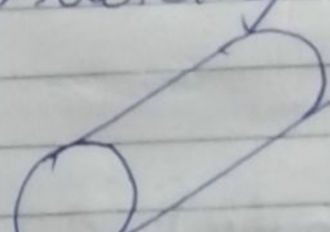
{Trivial soln} ↳ invalid soln.

Ground state: $\underline{n=1}$ $E \neq 0$
non-zero energy
⇓
non-zero velocity ⟵

$$\int_{-\infty}^{\infty} \psi^* \psi \, dx = 1 \quad \{\text{Normalization}\}$$

$$\int_0^a 4A^2 \sin^2 kx = 1$$

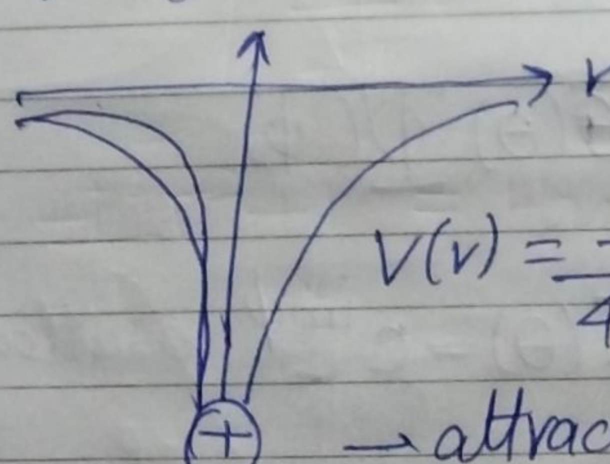
→ looking at the top of cylindrical box.



→ with higher energy, electron starts rotating.

⊖ →

Hydrogen Atom:-



$$V(r) = \frac{-Ze^2}{4\pi\epsilon_0 r} \quad \{\text{Calombic potential}\}$$

→ attractive potential from nuclei

→ potential is ~~xx~~ spherically symmetric

→ $\psi(r, \theta, \phi)$ → Univalued.

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$$\psi(r,\theta,\phi) = \psi(r,\theta,\phi+2\pi) = \cancel{\psi(r,\theta,\phi}$$

$$= \psi(r,\theta+2\pi,\phi)$$

→ periodic boundary conditions. (univalued)

$r \to \infty$, $\psi \to 0$

SE in three dimensions:-

$$\left[\frac{-\hbar^2}{2m}\nabla^2 + V\right]\psi = i\hbar\frac{\partial\psi}{\partial t} \qquad \nabla^2 = \frac{\partial^2}{\partial x^2}$$

In spherical coordinates.

$$\frac{-\hbar^2}{2m}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right)\right.$$

$$\left.+\frac{1}{r^2\sin^2\theta}\left(\frac{\partial^2\psi}{\partial\phi^2}\right)\right] = i\hbar\frac{\partial\psi}{\partial t}$$

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

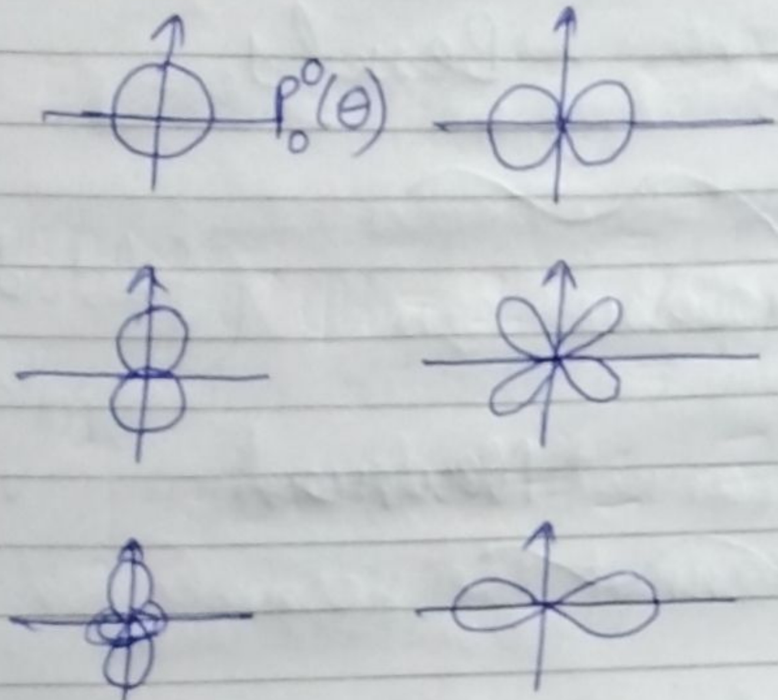
$$\frac{\partial^2\Phi}{\partial\phi^2} = -m^2\phi \Rightarrow \Phi(\theta) = e^{im\phi} \text{ oscillating}$$

$$\sin\theta\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\Theta}{\partial\theta}\right) + \left[l(l+1)\sin^2\theta - m^2\right]\Phi = 0$$

Solns are associated with Legendre polynomials.

$$P_\ell^m(x) = (1-x^2)^{\frac{|m|}{2}} \left(\frac{d}{dx}\right)^{|m|}$$

Associated Legendre's functionals P_ℓ^m



Radial:

$$\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) - \frac{2mr^2}{\hbar^2}\left(V(r)-E\right)R = \ell(\ell+1)R$$

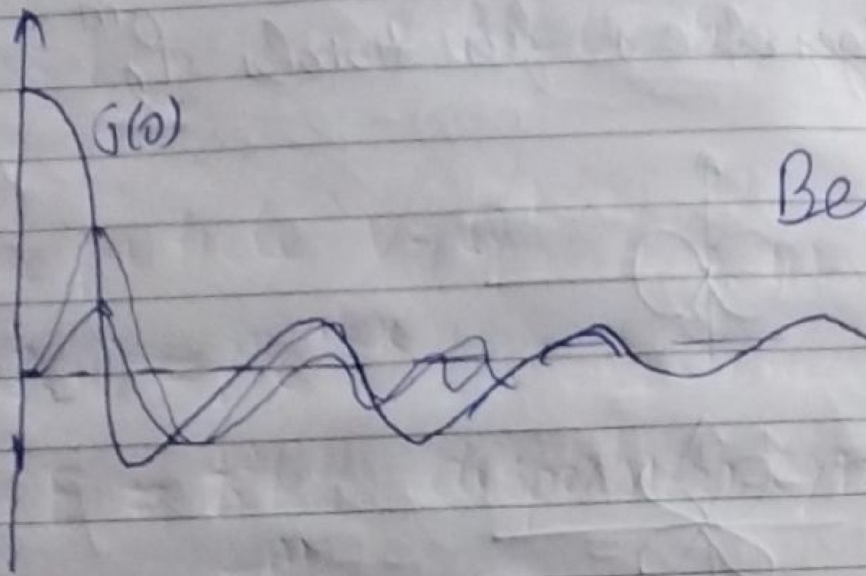
Introduce a new variable: $u = rR$

$$u(r) = Ar\,j_\ell(kr) + Br\,n_\ell(kr)$$

$j_\ell \Rightarrow$ spherical Bessel's function.

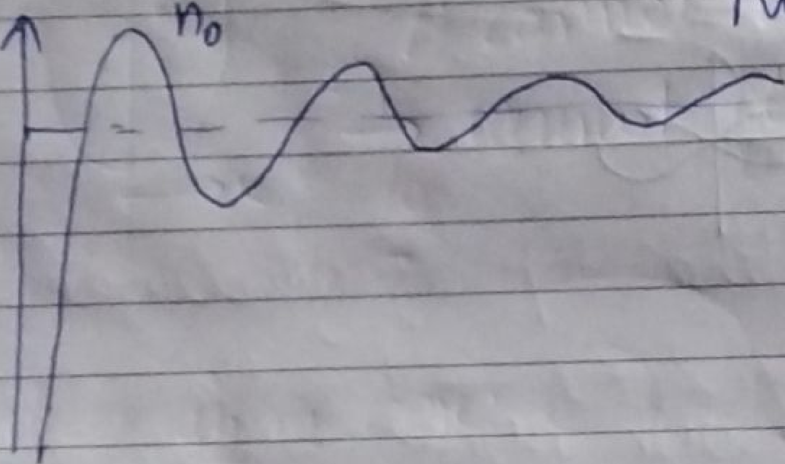
$n_\ell \Rightarrow$ spherical Neumann function.

Bessel's

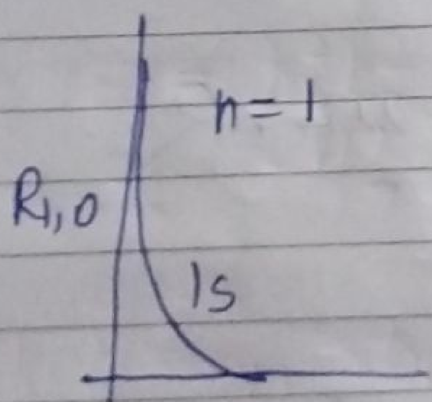


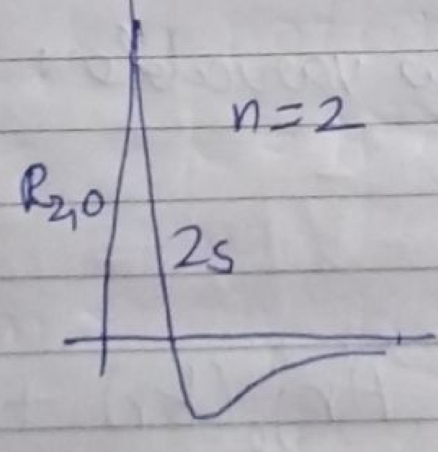
(falstad.com) orbital viewer

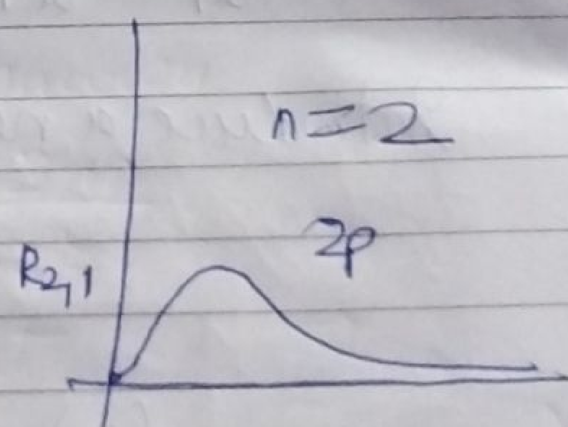
Neuman

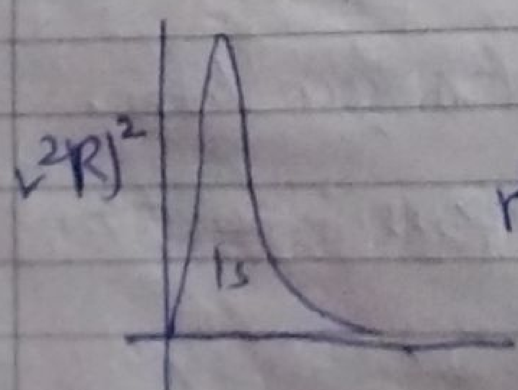


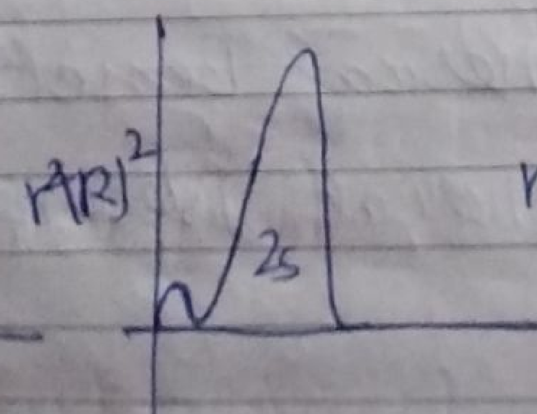
Radial Wavefunctions:

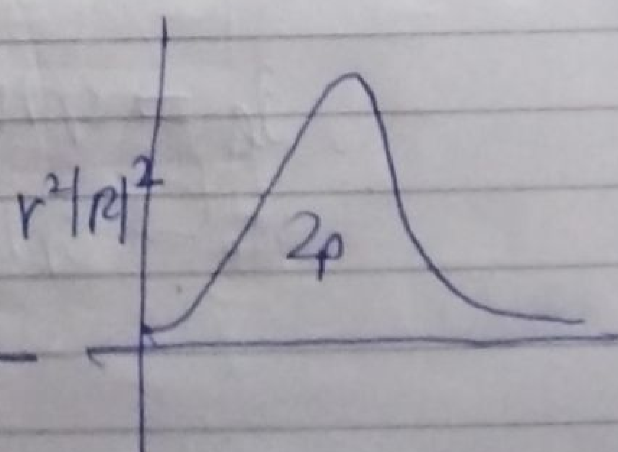












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Energy levels: Only radial dependence!

$$E_n = \frac{-Z^2 E_1}{n^2} \quad E_1 = \frac{me^4}{8\epsilon^2 h^2} = 13.6 eV$$

ground state energy of H atom.

→ higher quantum no. orbitals are degenerate.

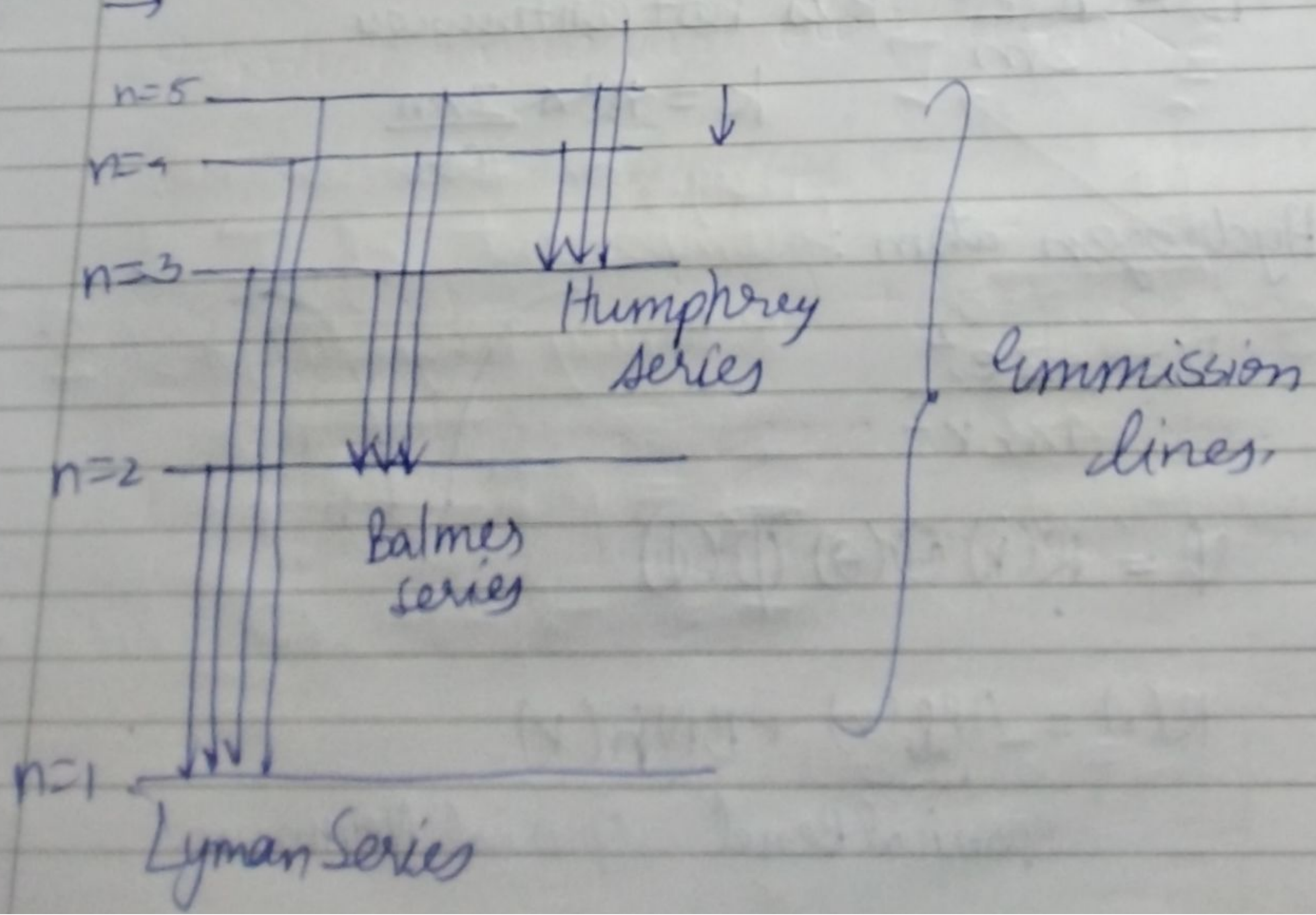
$$\psi = R(r)\,\Theta(\theta)\,\Phi(\phi)$$

$R(r) \to AJ_n(r)$, $\Theta(\theta) \to P^l(\theta)$, $\Phi(\phi) \to e^{-im\phi}$

→ discrete energy levels:

↳ discrete emmission ~~levels~~ lines in radiated spectrum.

→



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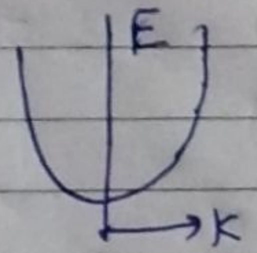
free particle: $V = 0$

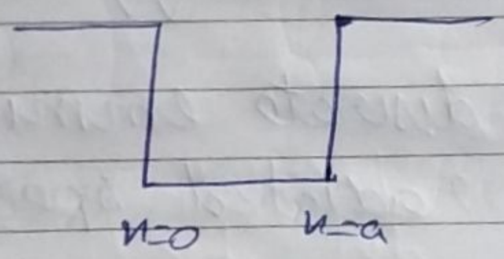
$\psi(x) = Ae^{ikx}$ $\quad k = \text{continuous} = \frac{2\pi}{\lambda}$

$E = \frac{\hbar^2 k^2}{2m}$ dispersion eqn



A cannot be found
→ cannot be normalized.

particle in a box:

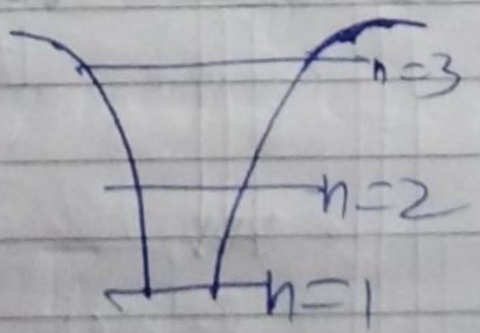


$\psi(x) = 2A_j \sin kx$

$E = \frac{\hbar^2 k^2}{2m}$ k is not continuous

$k = \cancel{\hbar 2\pi}\ \frac{2\pi n}{a}$

Hydrogen atom:



$V = \frac{-Ze^2}{4\pi\varepsilon r^2}$

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

$R(r) = A\underbrace{B_l(r)}_{\text{spherical Bessel}} + B\underbrace{N_n(r)}_{\text{spherical Neumann.}}$

$E = -\frac{13.6}{n^2} \cdot Z^2$ {Hydrogen like species}

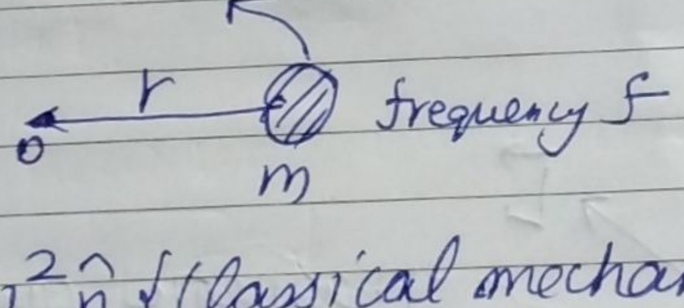
$\Theta_\ell \rightarrow$ Legendre's function.

$\phi_m \Rightarrow e^{im\theta}$

* State: energy levels that electrons can possibly take.

→ probability of finding electron at a particular (x, y, z) is univalued.

ANGULAR MOMENTUM:-



$\vec{L} = I_0 \omega^2 \hat{n}$ {Classical mechanics} $= mvr\hat{n}$

$\hat{H}\psi = E\psi$

$\underbrace{\left[-\frac{\hbar^2}{2m}\nabla^2 + V\right]}_{\text{Hamiltonian operator.}} \psi = \underset{\text{energy}}{E}\psi$

$\underset{\text{angular momentum operator.}}{\hat{L}}\psi = L\psi$

$\boxed{L = \hbar\sqrt{\ell(\ell+1)}}$

* $\ell = 0, 1, \dots n-1$

$n=1, l=0, m=0$ s orbital

spherically symmetry

$\boxed{L=0}$ ⇒ electron is not rotating in s orbital

→ it is there in a spherical volume with known probability.

$n=2, l=0$

↓

1 node radially

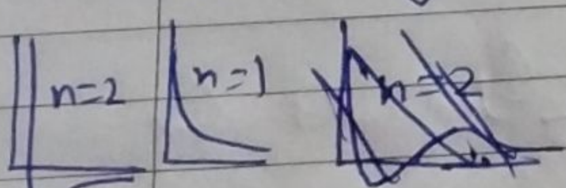
$l=1$

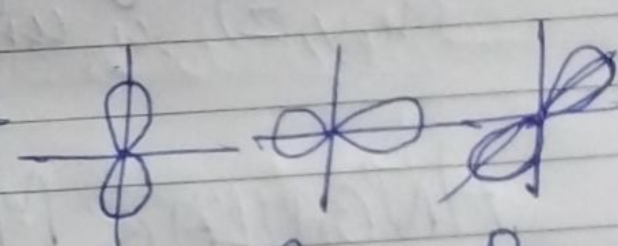
↓

1 node in θ

p orbital

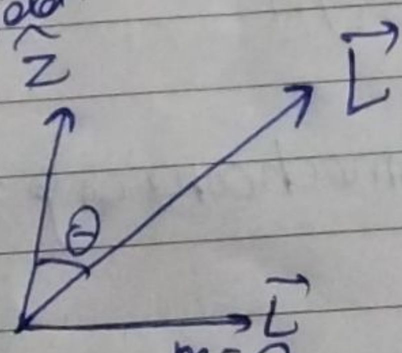
{dumbell axial symmetry}





P_y P_x P_z

arbitrary magnetic field.



$\hat{z}$ is quantized

hence θ is also quantised.

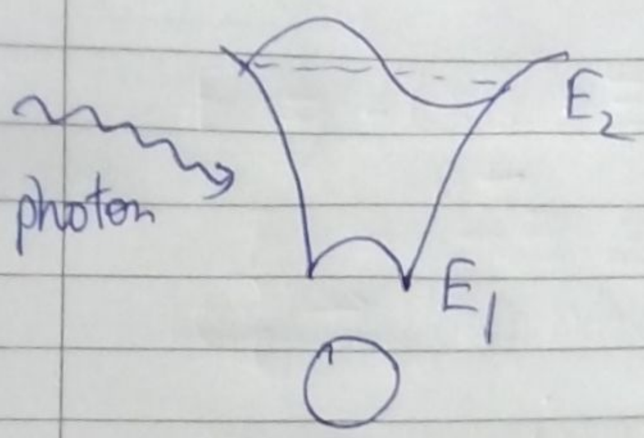
magnetic quantum no.

↳ component of $\vec{L}$ ~~at~~ along arbitrary magnetic field $\hat{z}$

$$\vec{L}_z = m\hbar$$

$$m = -l, -l+1 \ldots 0 \ldots 1, 2, \ldots l$$

$$L = \hbar\sqrt{l(l+1)}$$



$E_2 - E_1 = h\nu$

$\Delta l = 1$ {in absorption}

→ electron cannot be excited from s → s

→ has to excite from s ⟶ p

→ explains ~~Fraunhofer~~ atomic spectra lines.