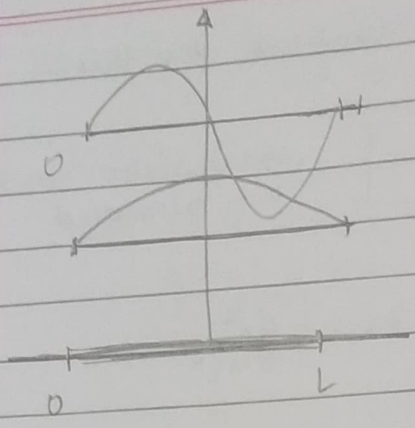
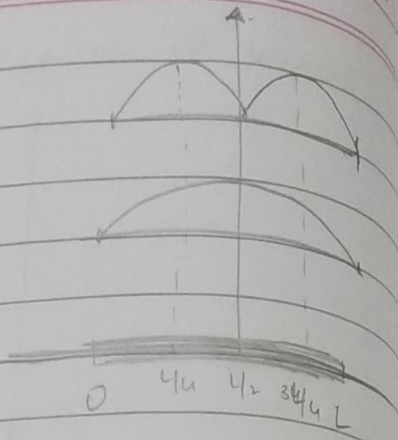
$\psi(x_1, y_1, z_1, x_2 y_2 z_2 \dots ; t) \rightarrow n$ particles

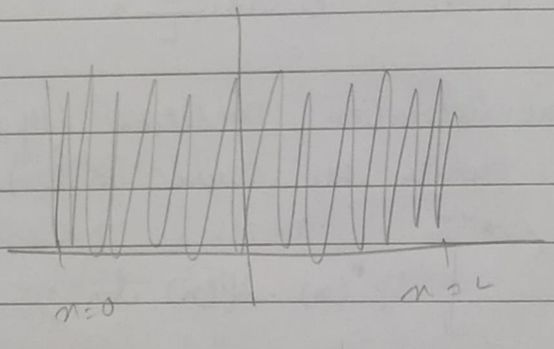




- Depending on the state, the probability of finding the particle varies
- As $n \uparrow$, probabilities becomes delocalized

As $n \rightarrow \infty$, all points are equally likely and thats when you hit the classical limit

Classical concepts revert when $n \rightarrow \infty$



- Recap:
  variable with ^ represents an operator
  All physical observables can be expressed as operators.

Eg: Momentum $\hat{P} = -i\hbar \frac{\partial}{\partial x}$

$i = \sqrt{-1}$ $\hbar = \frac{h}{2\pi}$

$h \rightarrow$ planks constant helps us move from classical to quantum mechanics. If $h \to 0$, we get back classical physics.

$$\hat{k} = \frac{-\hbar^2}{2m}\frac{\partial^2}{\partial x^2} = \frac{\hat{p}\cdot\hat{p}}{2m}$$

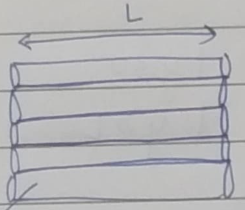
Now, $\hat{O}\,\Psi(x,t) = O\,\Psi(x,t)$

Scalar – measuring the mechanical property whose operator is $\hat{O}$

- Extension of 1D box model:

Take n wires & stack them on a plane.

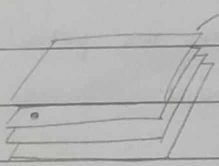
(1)



metallic film or sheet

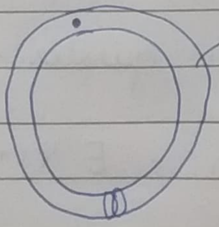
Graphene: one layer of C atoms

(2)



3D extension

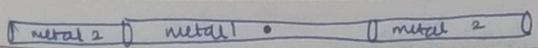
(3)



single wire / circular loop.

crude model (2D) of an atom

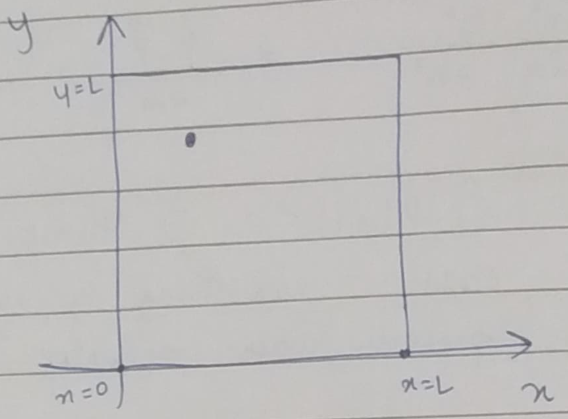
(4)



barrier is no longer ∞ at the ends

QM will change when the barrier is not ∞.

PARTICLE IN A 2D BOX:



As in the 1D case, the ē cannot go outside the film. The potential energy will now be a function of 2 variables

$$U(x,y) = \infty \qquad \begin{matrix} x \le 0 \mid y \le 0 \\ x \geq L \mid y \geq L \end{matrix}$$

$U(x,y) = 0$ (inside the film)

At a given (x,y) ψ tells you the probability of finding the ~~particle~~ ē at that point.

Inside the sheet :- $U(x,y) = 0$

Considering the 2D Schrodinger operator :-

$$-\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right]\psi(x,y) = E\,\psi(x,y)$$

Use $\psi(x,y) = X(x)\,Y(y)$.

[If X & Y are independent (uncoupled), their probabilities can be multiplied ... (unclear)]

$$Y(y)\left(\frac{-\hbar^2}{2m}\frac{\partial^2 X(x)}{\partial x^2}\right) + X(x)\left(\frac{-\hbar^2}{2m}\frac{\partial^2 Y(y)}{\partial y^2}\right) = \underbrace{E X(x) Y(y)}_{E_1 + E_2}$$

$\div$ by $X(x)\,Y(y)$ on both sides :-

$$\underbrace{\frac{1}{X(x)}\left(\frac{-\hbar^2}{2m}\frac{\partial^2 X(x)}{\partial x^2}\right)}_{E_1} + \underbrace{\frac{1}{Y(y)}\left(\frac{-\hbar^2}{2m}\frac{\partial^2 Y(y)}{\partial y^2}\right)}_{E_2} = E$$

?? $E_1 = \frac{n_1^2 h^2}{8mL^2}$ $\qquad$ $E_2 = \frac{n_2^2 h^2}{8mL^2}$.

$$E = E_1 + E_2 = \frac{(n_1^2 + n_2^2)\,h^2}{8mL^2}$$

Final wave function depends on 2 quantum no:s

$$\psi_{(n_1, n_2)}(x, y) = \frac{2}{L}\sin\left(\frac{n_1 \pi x}{L}\right)\sin\left(\frac{n_2 \pi y}{L}\right)$$

Ground state:-

$n_1 = n_2 = 1 \Rightarrow E_{11} = \frac{2h^2}{8mL^2}$

First excited $\left.\begin{array}{l} n_1 = 1,\ n_2 = 2 \\ n_1 = 2,\ n_2 = 1 \end{array}\right\} \Rightarrow E_{21} = E_{12} = \frac{5h^2}{8mL^2}$.

→ Degeneracy: 2 or more different quantum states having the same energy but all these are distinct states.

→ Particle in a 1-Dimensional box:- (Revisiting)

- Ground state $(n=1)$
  wave function $\psi_1(x) = \sqrt{\frac{2}{L}} \sin \frac{\pi x}{L}$

Calculate $\langle x \rangle$, $\langle x^2 \rangle$, $\langle p \rangle$, $\langle p^2 \rangle$

$$\langle (\Delta x)^2 \rangle = \langle x^2 \rangle - (\langle x \rangle)^2$$
$$\langle (\Delta p)^2 \rangle = \langle p^2 \rangle - (\langle p \rangle)^2$$

TIP:

$$\langle A \rangle = \int_x \psi^*(x)\, \hat{A}\, \psi(x)\, dx$$

If not normalized $\langle A \rangle = \dfrac{\int_x \psi^*(x)\, \hat{A}\, \psi(x)\, dx}{\int_x \psi^*(x)\psi(x)\, dx}$

~ Uncertainity principle:-
$\Delta x \Delta p \geq \hbar$

$$\langle x \rangle = \int_{\cancel{x}\, 0}^{L} x \cdot \frac{2}{L} \sin^2 \frac{\pi x}{L}\, dx.$$

$$= \frac{2}{L}\left[\int_0^L x \sin^2 \frac{\pi x}{L}\, dx\right] = \frac{2}{L}\left[\int_0^L x\left(\frac{1-\cos 2\pi x/L}{2}\right) dx\right]$$

$$= \frac{2}{L}\left[\int_0^L \frac{x}{2} - \frac{x \cos \frac{2\pi x}{L}\, dx}{2}\right]$$

$$= \frac{\cancel{2}}{\cancel{L}} \cdot \frac{L^{\cancel{2}}}{\cancel{4}\,2} - \frac{1}{L}\int_0^L x \cos \frac{2\pi x}{L}$$

$$= \frac{L}{2} - \frac{1}{L}\left[\cancel{\frac{x \cdot \sin 2\pi x/L}{\frac{1}{2\pi}}}_{0} - \frac{\sin 2\pi x}{1/2\pi}\right]_0^L$$

$$= \frac{L}{2}$$

classmate

Date

Page

And, $\langle x^2 \rangle = \int_0^L x^2 \sin^2 \frac{\pi x}{L}\, dx$

$= \cancel{\frac{L^3}{6}}$

$= \frac{L^2}{6}\left(2 - \frac{3}{\pi^2}\right)$

Further, $\langle p \rangle = \int \psi^*(x) \left(-i\hbar \frac{\partial}{\partial x} \psi(x)\right) dx$

P operate on ψ first & then with ψ^*

$= \int \sqrt{\frac{2}{L}} \sin \frac{\pi x}{L} \left(-i\hbar \frac{\partial}{\partial x} \sqrt{\frac{2}{L}} \sin \frac{\pi x}{L}\right) dx$

$= \int \sqrt{\frac{2}{L}} \sin \frac{\pi x}{L} \left(-i\hbar \sqrt{\frac{2}{L}} \cdot \cos \frac{\pi x}{L} \cdot \frac{\pi}{L}\right) dx.$

$= -\int \sqrt{\frac{2}{L}} \sin \frac{\pi x}{L} \cos \frac{\pi x}{L} \cdot \sqrt{\frac{2}{L}} \cdot \frac{\pi}{L} \cdot \frac{h}{2\pi} \cdot i \; dx$

$= -\int \frac{2}{L} \cdot \frac{h}{2\pi} \cdot \frac{\pi}{L} \cdot \sin \frac{\pi x}{L} \cos \frac{\pi x}{L}\; i\, dx$

$= -\int \frac{hi}{L^2} \sin\left(\frac{\pi x}{L}\right) \cos\left(\frac{\pi x}{L}\right) dx$

$= -\int \frac{hi}{2L^2} \sin\left(\frac{2\pi x}{L}\right) dx$

$= +\frac{hi}{2L^2} \cdot \left. \cos\left(\frac{2\pi x}{L}\right) \cdot \frac{L}{2\pi} \right|_0^L$

$= \hbar i/2L \; [1-1]$

$= \langle P \rangle = 0$

And, $\langle p^2 \rangle = \int_0^L \psi^*(x) \cdot -\hbar^2 \frac{\partial^2}{\partial x^2}\left(\sqrt{\frac{2}{L}} \sin \frac{\pi x}{L}\right) dx$

$= \int_0^L \sqrt{\frac{2}{L}} \sin \frac{\pi x}{L} \left(-\hbar^2\right) \frac{\partial}{\partial x}\left(\sqrt{\frac{2}{L}} \cdot \cos \frac{\pi x}{L} \cdot \frac{\pi}{L}\right) dx$

$= \int_0^L \sqrt{\frac{2}{L}} \cdot \sin\left(\frac{\pi x}{L}\right) \left(-h^2\right) \cdot \sqrt{\frac{2}{L}} \cdot \frac{\pi}{L} \cdot \left(\frac{-\sin \pi x}{L}\right) \pi x \; dx.$

$= \int_0^L \frac{2\pi}{L^2} \cdot \hbar^2 \cdot \pi x \cdot \sin^2 \frac{\pi x}{L}\, dx$

$= \frac{2\pi^2 \hbar^2}{L^2} \int_0^L x \sin^2 \frac{\pi x}{L} = \frac{2\pi^2 \hbar^2}{L^2} \cdot \frac{L}{2}$

$= \frac{\pi^2}{L} \cdot \frac{h^2}{4\pi^2} = \boxed{\frac{h^2}{4L^2}}$

lazer cooling.

- **Uncertainity in x & p**

$$\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$$

$$\Delta p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2}$$

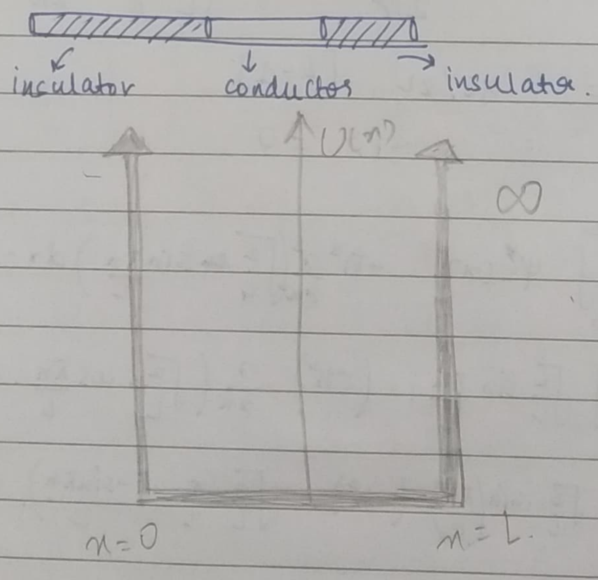
$$\boxed{\Delta x \Delta p \geq \hbar}$$ → Heinsenbergs uncertainty principle.

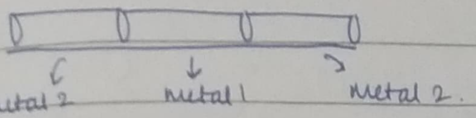
$\Delta x \Delta p > \hbar$ mostly

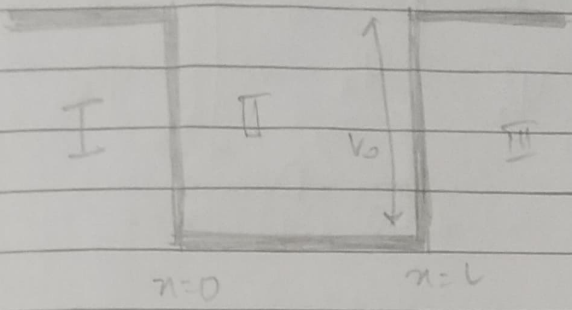
$\Delta x \Delta p = \hbar$ rarely

(Lazer cooling: dilute the system & use lazer light of diff wavelength. They increase the uncertainity of momentum of the particles as the 'frozen' atoms are subjected to radiations. The position can be accurately calculated ~~as~~ Atom can pick any momentum it wants. Resembles the atoms being frozen).

→ **Particle in an infinite well:**

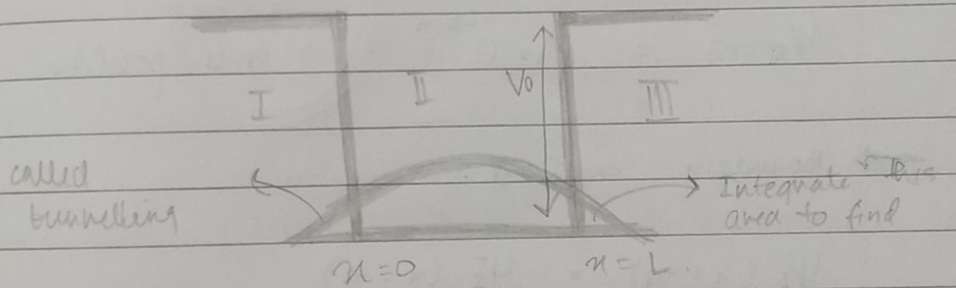






If the $\bar{e}$ is in II & has sufficient energy, it can cross the energy barrier & move to region I or III.
[Assumption Metal II more conducting than Metal I.]

when $E < V_0$ (stuck in the well)
! Classically you'd expect the P(find $\bar{e}$ in I / III) = 0
But quantum mechanics:- ψ is non zero



As you decrease the barrier ht, the probability of finding the quantum particle outside increases
∴ It is a function of V_0.

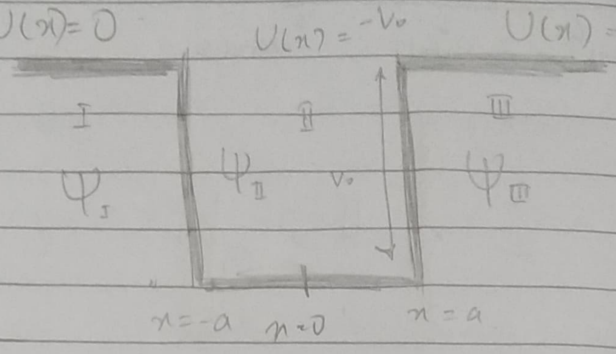
This is a simple model mimicing solids. Represents the $\bar{e}$ bounded to the nucleus, which if supplied with sufficient energy, Ionizes.

~ Quantum Tunnelling: penetration of probability to find the particle beyond II is called quantum tunnelling

→ Placing the tip of a metal wire close to the surface of metal, ∃ a small non zero prob of ē moving out of the well

→ Scanning tunnelling microscopy

0 axis



Region I : $U(x) = 0$

ie: $\dfrac{-\hbar^2}{2m} \dfrac{\partial^2}{\partial x^2} \psi_I(x) = E \psi(x)$

$\frac{d}{dx}\left(\frac{dy}{dx}\right)$

$\frac{d^2 y}{dx^2} = -ky$

$\psi_1(x) = C_1 e^{k_1 x}$ $\qquad k_1 = \sqrt{\dfrac{2m|E|}{\hbar^2}}$

exponentially decaying function

∵ k_1 is positive but x is is neg in region I

$\psi_{III}(x) = A_2 e^{-k_1 x}$ $\qquad x$ is positive

→ Boundary Conditions :

$\psi_I(x = -a) = \psi_{II}(x = -a)$

- ψ should be single valued

$\dfrac{d}{dx}\psi_I = \dfrac{d}{dx}\psi_{II}$ [Avoid momentum discontinuity ∵ $\frac{d}{dx}\psi(x)$ = Momentum

∴ • ψ is continuous .

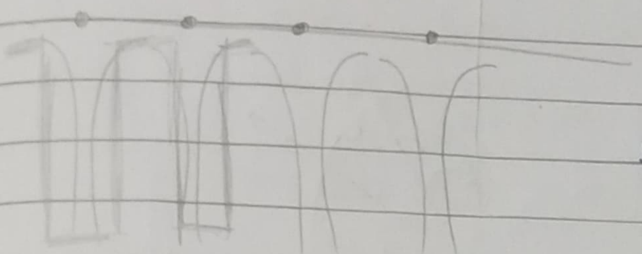
Similarly :

$\psi_{II}(x = a) = \psi_{III}(x = a)$

$\dfrac{d}{dx}(\psi_{II}(x = a)) = \dfrac{d}{dx}\psi_{III}(x = a)$

→ Helps understand band-gaps.

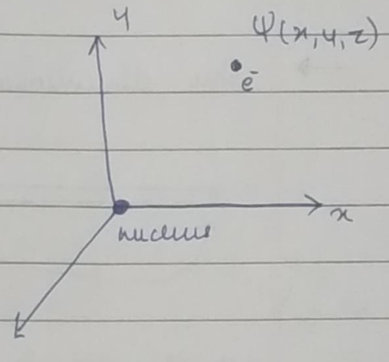
Q: Consider a ~~Q~~ 1-D solid : periodic array of atoms
calculate the interaction b/w $\bar{e}$ & nucleus



series of wells.

Potential barrier : ionization energy

- ATOMS:



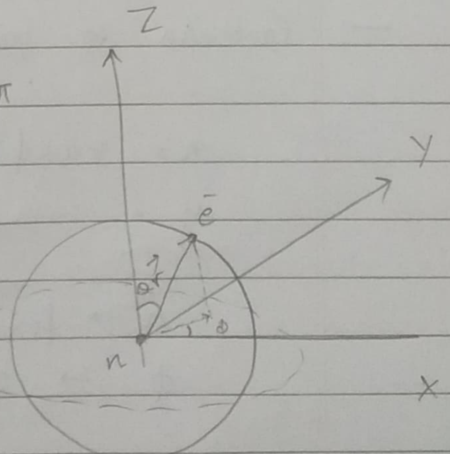
$\psi(x,y,z)$ represents the electron cloud.

$\psi(x,y,z)\ \psi^*(x,y,z)$.
→ probability density of electron at (x,y,z)

Now here $U(x,y,z) \neq 0$ ∵ the $\bar{e}$ interacts with the nucleus.
For mathematical simplicity convert from cartesian to polar coordinates. (Rotational degrees of freedom).

$$\psi(x,y,z) \longrightarrow \psi(r,\theta,\phi)$$

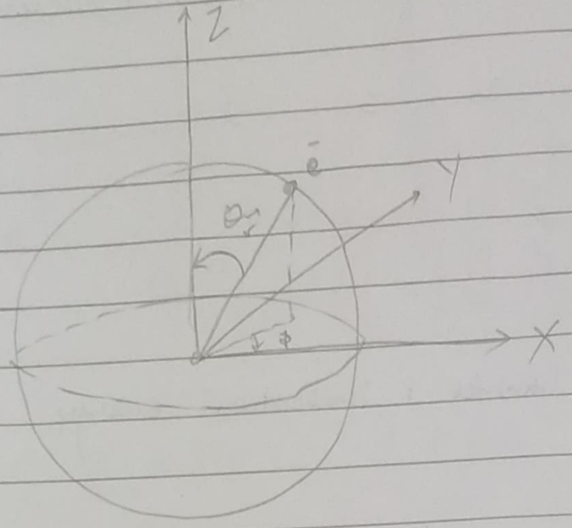
- ϕ: angle that projection of $\vec{r}$ makes with the x-axis $\theta \to 0$ to π
  ϕ: $0 - 2\pi$.
- θ: angle $\vec{r}$ makes with z-axis
  θ : $0 - 2\pi$
- $\vec{r}$: $0 - \infty$



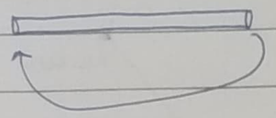
Generate all possible points on surface of sphere. Prevent double counting 2π

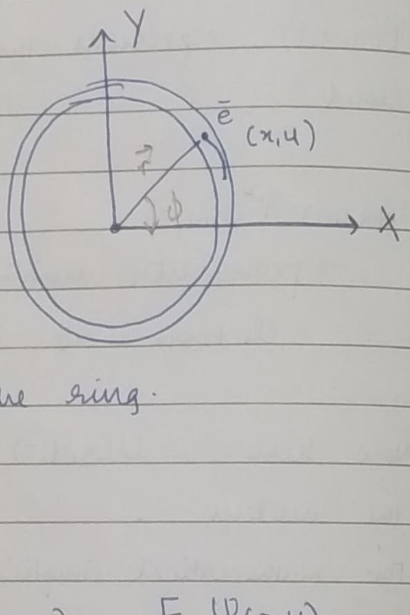
Overlap ⇒ Chemical bonds

Using this we'll explain the orbitals 1s, 2s, 2p...



→ One dimensional atom :-





For an atom, its free through space (3D) unlike here 2D

Let this $\bar{e}$ be a free electron ⇒ $U(x,y) = 0$

Freely moving along the ring.

∴ Schrodinger Eqn :-

$$-\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right]\psi(x,y) = E\,\psi(x,y).$$

— Cartesian to polar coordinates:-

$\frac{\partial}{\partial x}$ = $-r\sin\phi$.. $r\cos\phi$ -rsi

$x = r\cos\phi$

$y = r\sin\phi$

$r \rightarrow$ fixed

$\phi \rightarrow 0$ to 2π.

* $\psi(r,\phi) = R(r)\,\Phi(\phi)$ ... variable separable

And, $\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} = \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{\partial^2}{\partial \phi^2}$

Note:- for any function $f(x,y)$.

$$\frac{\partial f(x,y)}{\partial r} = \frac{\partial f}{\partial x}\cdot\frac{\partial x}{\partial r} + \frac{\partial f}{\partial y}\cdot\frac{\partial y}{\partial r}$$

$$\frac{\partial f}{\partial x}\cdot\cos\phi + \frac{\partial f}{\partial y}\sin\phi$$

Now since r is fixed $\frac{\partial^2}{\partial r^2} = 0 = \frac{\partial}{\partial r}$

$\therefore$ $\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} = \frac{\partial^2}{\partial \phi^2}$ ---- essentially 1D (boils down)

$\Rightarrow$ Schrodinger eqn in Polar coordinates

$$-\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{\partial^2}{\partial \phi^2}\cdot\psi(r,\phi) = E(\psi(r,\phi))$$

* Since we are interested only in the angular part of the wave function :- LHS & RHS r component cancels out.

$$\Rightarrow \quad -\frac{\hbar^2}{2m}\frac{1}{r^2}\frac{\partial^2}{\partial \phi^2}\cdot\Phi(\phi) = E\,\Phi(\phi)$$

Also, $I = mr^2$ ... moment of inertia

$\therefore$

$$\Rightarrow \quad -\frac{\hbar^2}{2I}\frac{\partial^2}{\partial \phi^2}\Phi(\phi) = E\,\Phi(\phi).$$

$$\Rightarrow \quad \frac{\partial^2}{\partial \phi^2}\Phi(\phi) = -\frac{2IE\,\Phi(\phi)}{\hbar^2} \quad \ldots \text{SHM}$$

General solution:-

$$\Phi(\phi) = Ae^{im\phi}$$

Applying boundary conditions [ψ should be single valued]

$$\Phi(\phi + 2\pi) = \Phi(\phi)$$

$$A e^{i m_l (\phi + 2\pi)} = A e^{i m_l \phi}$$

$$e^{i m_l 2\pi} = 1$$

$$m_l = 0, \pm 1, \pm 2 \dots$$

m_l :- magnetic quantum number

Substitute $\Phi(\phi) = A e^{i m_l \phi}$ in the schrodinger eqn. and determine E.

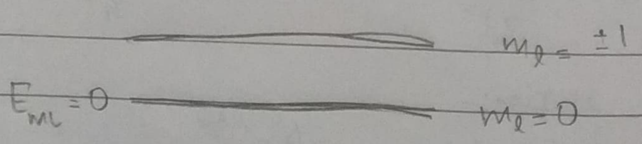
(m_l) determines state of the electron.

$$\Rightarrow \boxed{E_{m_l} = \frac{m_l^2 \hbar^2}{2I}} \qquad m_l = 0, \pm 1, \pm 2 \dots$$

When $m_l = 0$, wave function is a constant

but $m_l = 0 \Rightarrow E = 0$

ψ is a straight flat line [$\because$ second derivative WRT ϕ] $\Rightarrow$ Kinetic energy $= 0$



① polar cood.
② ∇^2
③ Schrodinger eqn in polar Cood
④ Apply the boundary Condition

To calculate A : Normalise the wave function

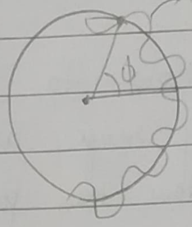
$$\Phi(\phi) = A e^{i m_l \phi}$$

ie: $$\int_0^{2\pi} \Phi^*(\phi)\, \Phi(\phi)\, d\phi = 1.$$

$$\boxed{A = \frac{1}{\sqrt{2\pi}}}$$

∴ For an $\bar{e}$ in a ring,

$$\Phi(\phi) = \frac{1}{\sqrt{2\pi}} e^{i m_l \phi} \qquad m_l = 0, \pm 1, \pm 2 \ldots$$



→ Angular Momentum :

$$\vec{L} = \vec{r} \times \vec{P}$$

$$L_x \hat{i} + L_y \hat{j} + L_z \hat{k} = \begin{vmatrix} i & j & k \\ x & y & z \\ P_x & P_y & P_z \end{vmatrix}$$

$$L_z = x P_y - y P_x$$

$$\hat{L}_z = \hat{x}\left(-i\hbar \frac{\partial}{\partial y}\right) - \hat{y}\left(-i\hbar \frac{\partial}{\partial x}\right)$$

In polar :-

$$\hat{L}_z = \frac{\hbar}{i} \frac{\partial}{\partial \phi}$$

∴ $$\hat{L}_z \Phi(\phi) = \Phi(\phi)$$

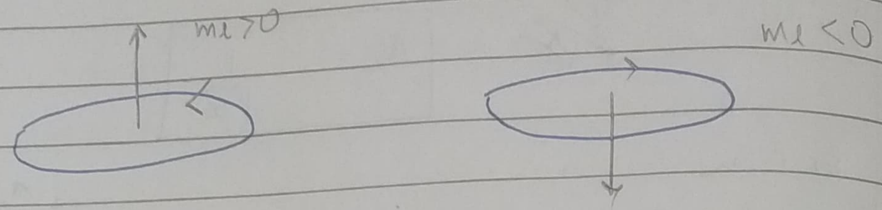
$$\frac{\hbar}{i} \frac{\partial}{\partial \phi}\left(A e^{i m_l \phi}\right)$$

$$= \frac{\hbar}{i}\, i m_l A e^{i m_l \phi} = \hbar m_l \Phi(\phi)$$

⇒ Angular momentum $= \hbar m_l$
↳ quantized ∵ $m_l = 0, \pm 1, \pm 2$

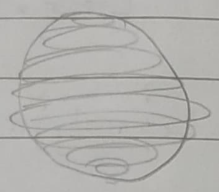
For a particle moving on a ring Engergy & angular momentum are quantized

m_l can be + or − . ∴, In reality :



Spin of ēs is related to the angular momentum (spin up / spin down)

- Now to generalize for 3D, consider a stack of rings as follows:
  Now the particle is on a sphere more relevant to the atomic model.



→ Particle on a sphere :

2 Degrees of freedom ⇒ 2 quantum no:

$r \rightarrow$ fixed.

$\phi \rightarrow 0$ to 2π (for any given region)

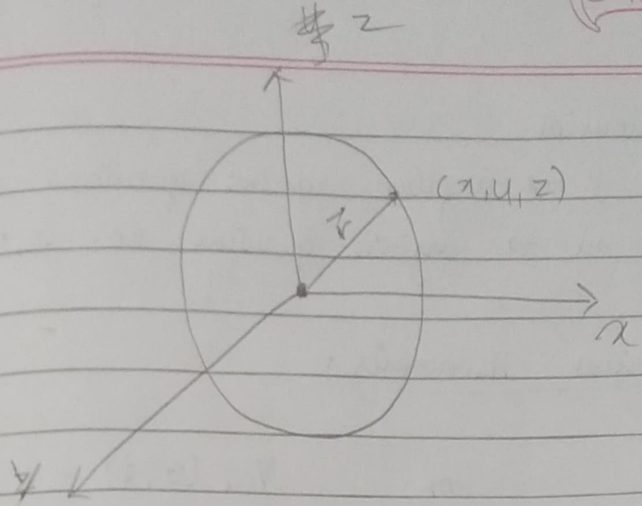
$\theta \rightarrow 0$ to π

l: angular moment quantum no: $= 0, 1, 2, \ldots$

$m_l = 0, \pm 1, \pm 2 \ldots \ldots \pm l$ $= ?$

Building the schrodinger eqn:-

$$\frac{-\hbar^2}{2m}\left[\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right]\psi(x,y,z) = E\,\psi(x,y,z)$$



converting cartesian to spherical polar coordinates:-

$$x = r\sin\theta\cos\phi$$

$$y = r\sin\theta\sin\phi$$

$$z = r\cos\theta .$$

Step 1: Express $\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ in terms of r, θ, ϕ

$$\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\Lambda^2$$

where

$$\Lambda^2 \equiv \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial \phi^2} + \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)$$

Step 2: Schrodinger equation

wave function... $Y_{lm}(\theta, \phi)$

with only angular part

$$\Lambda^2\psi(r,\theta,\phi) = -\left(\frac{2IE}{\hbar^2}\right)\psi(r,\theta,\phi)$$

$Y_{lm}(\theta, \phi)$

$I = mr^2$ ... moment of inertia.

Solution: spherical harmonics $Y_{lm}(\theta, \phi)$ → probability of finding the $\bar{e}$ at the point θ, ϕ

↳ 2 quantum no:s l, m.

$$Y_{lm}(\theta,\phi) = \sqrt{\frac{(2l+1)}{4\pi}\frac{(l-m)!}{(l+m)!}}\; P_{lm}\cos\theta\, e^{im\phi}$$

Here $P_{lm}(\cos\theta)$ is called the associated legendre

All wave functions are normalized

polynomial.

$l \rightarrow$ angular moment quantum no: $(0, 1, 2 \ldots)$

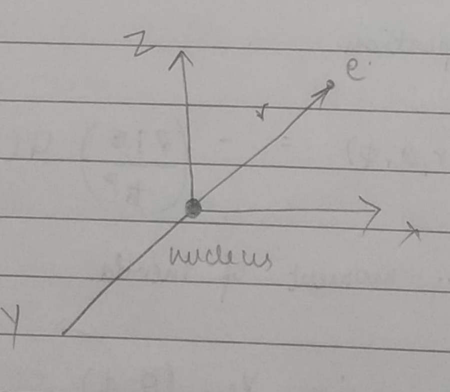
$m \rightarrow$ magnetic quantum no: $(0, \pm 1, \pm 2 \ldots \pm l)$

→ Spherical Harmonics :

l	m	$Y_{lm}(\theta, \phi)$	
equal probability → 0	0	$\frac{1}{2}\sqrt{\pi}$	... constant
1	0	$\frac{1}{2}\sqrt{3\pi}\cos\theta$	
1	± 1	$\mp\sqrt{\frac{3}{2\pi}}\sin\theta\, e^{\pm i\phi}$	

For $l = 0$, $m = 0$ when equal probabilities of finding the $\bar{e}$ for whatever θ, ϕ. These orbitals are called spherical orbitals ⟶ s orbitals

- HYDROGEN ATOM (not confined in ring/ sphere)



All r, θ, ϕ vary

$$U(r) = \frac{-1}{4\pi\epsilon_0}\frac{e^2}{r}$$ ... Coulomb's law

Again :

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$ use r, θ, ϕ

All linear P.D.E ⇒ variable separable works
Quantum mech → all linear
Homog - Entire eqn = 0

K.E.

$$\Rightarrow \boxed{-\frac{\hbar^2}{2m}\left(\frac{\partial}{\partial r}\underbrace{\left(r^2\frac{\partial}{\partial r}\right)}_{radial}\right)\psi(r,\theta,\phi) - \frac{\hbar^2}{2m}\underbrace{\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right)}_{angular}\psi(r,\theta,\phi)}$$

P.E ⇐ $\boxed{-\frac{e^2}{4\pi\epsilon_0 r}\psi(r,\theta,\phi)} = E\,\psi(r,\theta,\phi)$.

By Method of Separation: $\psi(r,\theta,\phi) = \underbrace{R(r)}_{\text{radial part}} \cdot \underbrace{Y(r,\theta,\phi)}_{\text{angular part}}$.

$$\Rightarrow -\frac{\hbar^2}{2m}\underbrace{Y(\theta,\phi)}_{\text{angular part}}\left(\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}R(r)\right)\right)$$

radial part (including potential energy) $+E\psi($ cons

radial part + angular part = 0
equate to C | equate to −C
use particle on a sphere model

Solution of the angular part } from particle on a sphere

Radial part :- $R_{nl}(r)$

We have three quantum numbers :-

$n = 1, 2, 3 \ldots$

$l = 0, 1, 2 \ldots n-1$

$m = 0, \pm 1, \pm 2 \ldots \pm l$

$$\psi_{nlm}(r,\theta,\phi) = R_{nl}(\theta)\,Y_{lm}(\theta,\phi)$$

$l=0$ s $\quad$ $l=1$ - p orbital

	n	l	m	ψ
• 1s	1	0	0	$\psi_{100} = \frac{1}{\sqrt{\pi}}\left(\frac{1}{a}\right)^{3/2} e^{-\sigma}$

~~Varies with~~ Depends only on r

Prob over all θ, φ is same

$\sigma = \frac{r}{a_0}$; a_0 : Bohr's Radius.

	n	l	m	
• Indep of θ, φ	2	0	0	$\psi_{200} \propto \sigma e^{-\sigma/2}$ → 2s
• p_x, p_y, p_z	2	1	0	θ dependence, r
•	2	1	± 1	
•	2	1	-1	

→ For Radial prob. distribution

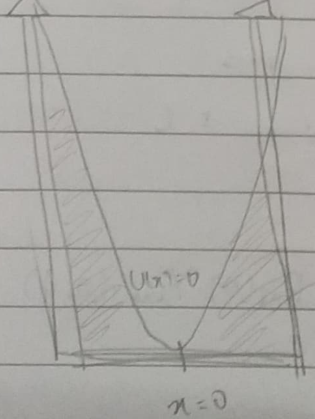
Spherical shell of thickness dr

Vol = $dV = 4\pi r^2 dr$; Density $|\psi^2| dV = |\psi^2| 4\pi r^2 dr$

$$P_r = \frac{4r^2}{r_0^3} e^{-\frac{2r}{r_0}} = 4\pi r^2 |\psi|^2$$

$$= 4\pi r^2 \times \frac{1}{\pi} \frac{1}{r_0^3} e^{-\frac{2r}{a_0}}$$

→ Unlike the previous case of atom in an infinite box, now ∃ a potential inside



→ quantum ~~mechanical~~ region

$U(x) = \frac{1}{2} k x^2$

$\omega = \sqrt{\frac{k}{m}}$.

To check whether normalised $\int = 1$

To check orthogonality $\int \psi_1 \psi_2 = 0$

For translational model - particle in a box is apt

rotational model - harmonic oscillator

In order to mimic the particle in a box problem, we must pick a small value for k. ∴, As $k \to 0$ it looks like the particle in a box