

Matrix Multiplication

Physics - 5

- Not Commutative $AB \neq BA$
- Associative $A(BC) = (AB)C$
- Distributive $A(B+C) = AB + AC$
- $\det(AB) = \det(A) \det(B)$
- $((AB)C)D = (A(BC))D = A((BC)D) = \dots$

[as long as you
preserve the order]

- Complex Conjugate :- Complex Conjugate of each element.

or

Conjugate Matrix

$$A_1 = \bar{A}$$

Conjugate Transpose = $(\bar{A})^T = \overline{(A^T)}$
(for Hermitian Operators)

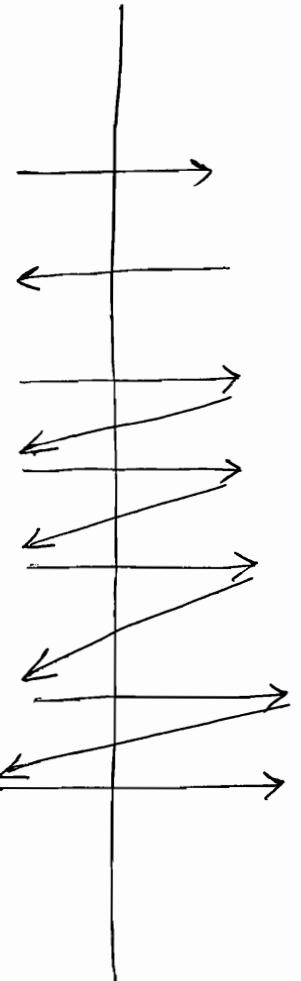
★ Proof of Heisenberg : end of lecture 2

★ Proof of H atom : end of notes

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dayslectures

| | |
|---|-------------|
| 2 | 1 |
| | 2 |
| | 3, 4 |
| 3 | 5 |
| | 6, 7, 8, 13 |
| 2 | 9, 10, 11 |
| | 12 |

Chapters (Verma)1, 2, 3
↓
4, 5

6, 7, 8, 9, 10, 11

12

13, 14, 15, 16, 17

18, 19

20, 21

① $\delta(x^2 - a^2) = \delta((x-a)(x+a)) = \frac{1}{2a} [\delta(x-a) + \delta(x+a)]$

② $(\nabla^2 + k^2) \frac{e^{ika}}{k} = -4\pi \delta(\vec{x})$

③ $\int_{-\infty}^{\infty} f(x) \delta'(x-a) dx = -f'(a)$

④ define $\delta(\vec{x}-\vec{x}') = \delta(x-x') \cdot \delta(y-y') \cdot \delta(z-z')$

& $\iiint f(\vec{r}) \delta(\vec{r}-\vec{r}') d\vec{r} = f(\vec{r}')$

Physics Paper (2)

Section A

① Quantum Mechanics (12)

② Atomic & Molecular Physics (10)

Section B

① Nuclear & Particle Physics

② Solid State Physics & Electronics

Quantum Mechanics

i) Basic Concepts (Preliminaries)

- Wave Particle duality
- Heisenberg's Uncertainty Principle
- Axioms of Quantum Mechanics

(Eigenvalues, Eigen Functions & Expectation values)

- Gaussian Wave Packet treatment of free particles

2) Eigen Values Problems

- Measurement of Energy

(Schrodinger's Wave Equation)

(Infinite Potential well)

- (i) Particle in 1-d / 3-d Box
- (ii) Particle in a finite well
- (iii) Step Potential
 - Reflection
 - Transmission

(in Rectangular Barrier)

3) E.V. problem of Angular Momentum. Measurement

- Orbital Angular Momentum

(in Simple Harmonic Oscillator)

- Spin Angular Momentum

(vi) H atom problem

(Pauli Spin Matrices)

(4) Miscellaneous

- density of states

- free electron theory of Metals

→ A particle showing dual behaviour shows only 1 behaviour at a particular time. This is called Principle of Complementarity.

Wave Particle Duality

De Broglie's Concept of Material Waves

→ Light exhibits dual behaviour, we know from interference and photoelectric effect.

$$E^2 = (\beta c)^2 + (m_0 c^2)^2$$

$$\text{For photons, } m_0 = 0 \Rightarrow E = \beta c \Rightarrow \beta = \left(\frac{E}{c} \right)$$

Planck said energy is quantized, $E = h\nu$

$$\Rightarrow \beta = \frac{h\nu}{c} = \left(\frac{h}{\lambda} \right) \quad \begin{matrix} \uparrow \\ \text{particle} \\ \text{property} \end{matrix} \quad \begin{matrix} \downarrow \\ \text{wave} \\ \text{property} \end{matrix} \quad \Rightarrow \lambda = \left(\frac{h}{\beta} \right)$$

De Broglie generalized that if photons are showing dual behaviour, similarly, all material particle show dual behaviour s.t. their $\lambda = \frac{h}{\beta} = \left(\frac{h}{m_0 v} \right)$

It was hypothesis. It was confirmed experimentally by Davisson - Germer and thus became De Broglie's Wave-Particle duality theory.

$$\vec{p} = \hbar \vec{k}$$

④ hypothesis $\xrightarrow{\text{experimental verification}}$ theory

$$\beta = \frac{h \cdot 2\pi}{\lambda \cdot 2\pi} = \frac{h}{(\lambda/2\pi)} = \hbar k$$

$$\lambda = \frac{h}{p} = \frac{h}{\sqrt{2mE}}$$

(non-relativistic energy)

[$p = \sqrt{2mE}$ Only for non-relativistic case]

we know $E = \frac{f}{2} kT$

\Rightarrow

$$\lambda = \frac{h}{\sqrt{mfkT}}$$

Q/ λ of neutron at 300K = $\frac{h}{\sqrt{3mkT}}$ (since $f=3$)

For thermal neutron, $f=2$

Q/ Energy of $e^- = 1 \text{ keV}$

$$\lambda = \frac{h}{\sqrt{2mE}}$$

$$\lambda = \frac{hc}{pc} = \frac{hc}{\sqrt{E^2 - m.c^2}}$$

(Since $E >$ rest mass energy, it is Relativistic Energy)
 [For e^- : $m.c^2 = 0.51 \text{ MeV}$]

Q/ λ Cricket Ball

Assuming critical ball to be particle

$$1 \text{ kg}, 180 \text{ km/hr} = 180 \times \frac{5}{18} = 50 \text{ m/s}$$

$$\lambda = \frac{h}{mv} = \frac{6.62 \times 10^{-34}}{1 \times 50} = \frac{13.24 \times 10^{-36}}{} \text{ m}$$

This wavelength is so small that we do not have any instrument to measure such a small wavelength.

Q/ e- mass : 9.1×10^{-31} kg
 $v = 10^6$ m/s (non relativistic)

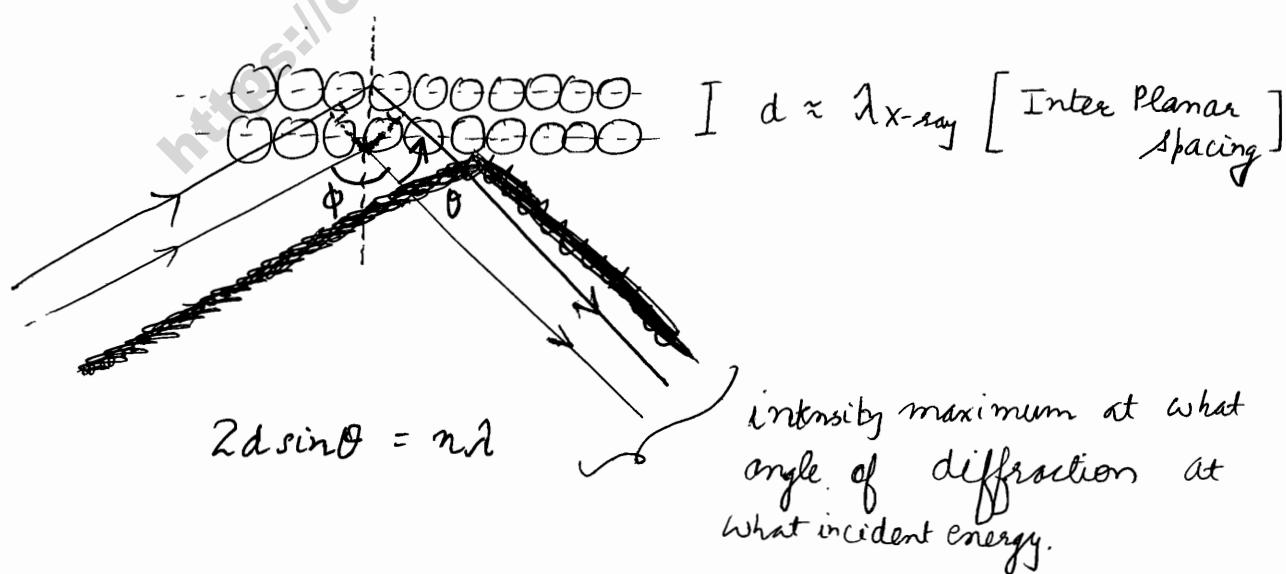
$$\lambda = \frac{h}{mv} = \frac{6.62 \times 10^{-34}}{9.1 \times 10^{-31} \times 10^6} \approx 7.3 \times 10^{-10}$$

We have instruments to measure λ upto 10^{-9} m easily.
Hence observable wave nature.

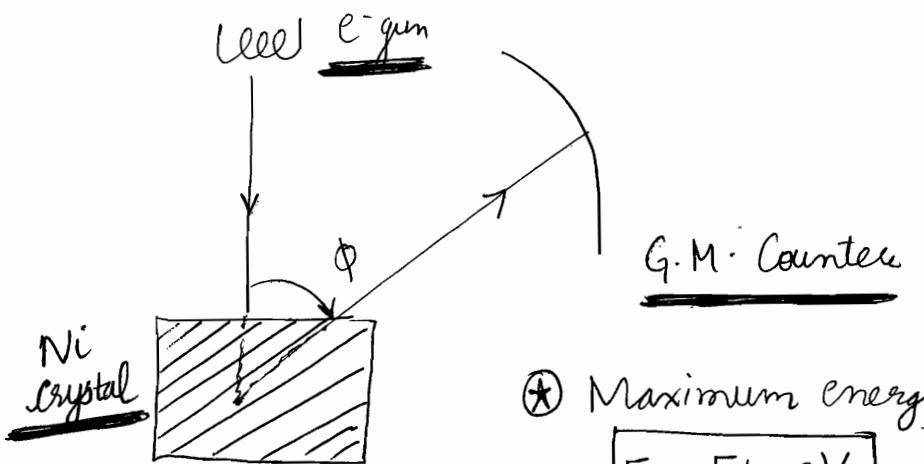
We can prove wave nature of particles, if we can show diffraction or interference in electrons.

Problem is to find a diffracting obstacle which has wavelength comparable to an electron.
light had wavelength ≈ 4000 Å but here the wavelength of e- is very less

X-rays have wavelength 0.1 to 1 Å. Diffraction of X-rays made possible using crystal arrangement of atoms.



- ① Garibaldi : unification of Italy (1850)
- ② Grimaldi : diffraction (1650)



G.M. Counter

★ Maximum energy/intensity
observed for,

- $E = 54 \text{ eV}$
- $\phi = 50^\circ$

Assuming validity of wave-particle duality:

$$\lambda = \frac{h}{\sqrt{2mE}}$$

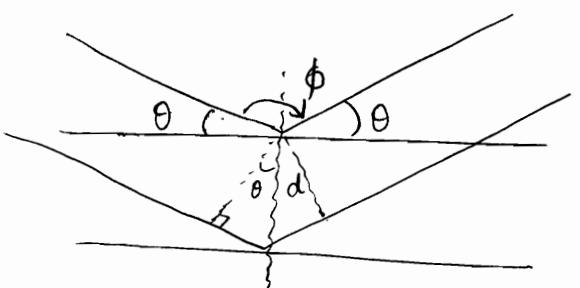
$$= \frac{6.6 \times 10^{-34}}{\sqrt{2 \times 9.1 \times 10^{-31} \times 54 \times 1.6 \times 10^{-19}}}$$

$$= 1.66 \text{ \AA}$$

$$= \frac{6.6 \times 10^{-34}}{9.49 \times 10^{-25}} =$$

$$= 0.166 \times 10^{-9}$$

Bragg's law for diffraction



$$\Delta = 2d \sin \theta$$

$$2d \sin \theta = n\lambda \text{ for maxima}$$

For 1st Maxima,

$$2d \sin \theta = \lambda$$

$$\odot 2\theta = (\pi - \phi)$$

$$\theta = \frac{130}{2} = 65^\circ$$

For Ni Crystal : $d = 0.92 \text{ \AA}$

$$\lambda = 2 \times 0.92 \times \sin 65^\circ$$

$$= 1.66 \text{ \AA}$$

Hence λ comes out to be same. Hence Wave-Particle duality confirmed for electrons.

We know

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

valid

$$\Rightarrow v_p = \frac{h\omega}{hk} = \frac{E}{p} = \frac{\frac{1}{2}mv^2}{mv} \quad (\text{non-relativistic})$$

(for material waves)

$$v_p = \left(\frac{\pi}{2} \right)$$

* These two expressions do not converge as in the 1st case, we have taken only k.e. while in the 2nd case, we have taken total energy

$$v_p = \frac{E}{p} = \frac{mc^2}{mv} \Rightarrow v_p = \left(\frac{c^2}{v} \right) \quad (\text{relativistic})$$

[STR is not violated as the particle is not moving with v_p]

$$v_g = \frac{dk}{dt} = \frac{h}{t} \frac{dw}{dk} = \frac{dE}{dp} = \frac{c^2 p}{E} = \frac{c^2 m v}{mc^2} = v$$

$$E^2 = p^2 c^2 + (m_0 c^2)^2 \Rightarrow 2E dE = 2p c^2 dp$$

$$\Rightarrow v_g = v$$

→ Remember that no matter relativistic or non-relativistic case, $p = mv$ is valid.

Hence particle is not like a monochromatic wave. It is like a wave packet or wave group.

We can also write,

$$\lambda = \frac{h}{p} = \frac{hc}{\sqrt{T^2 + 2Tm_0c^2}}$$

Note that it points towards HUP

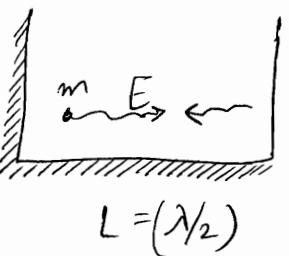
$$(T + m_0 c^2)^2 = (p c)^2 + (m_0 c^2)^2$$

$$\begin{aligned} \text{Total expression} &= \frac{\frac{1}{2}m_0 v^2 + m_0 c^2}{mv} \\ &= \frac{c^2}{v} \left[m_0 + \frac{m_0 u^2}{2c^2} \right] \\ &\approx \left(\frac{c^2}{v} \right) \end{aligned}$$

1-d Box



Motion in a straight line



→ Quantization of energy is inherent in de Broglie's theory

$$E = \frac{p^2}{2m}$$

(non-relativistic)

Standing Waves will form.

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



No hindrance

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



1 hindrance

$$L = \frac{3\lambda}{2}$$



2 hindrance

$$\Rightarrow L = \frac{n\lambda}{2} \Rightarrow \lambda_n = \left(\frac{2L}{n} \right)$$

→ n cannot be 0

Note that we can observe HOP from here $\Delta p \cdot \Delta x \leq \frac{h}{2L}$

$$\approx \left(\frac{h}{2L} \right)$$

$$p_n = \frac{h}{\lambda_n} = n \frac{h}{2L}$$

(Momentum is discrete)

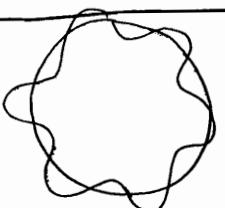
We use $E = \frac{p^2}{2m}$ as $E = T + V = T (V=0) \approx \left(\frac{p^2}{2m} \right)$ for non-relativistic case

$$E_n = n^2 \left(\frac{h^2}{8mL^2} \right) \quad n = 1, 2, 3, \dots$$

Hence, particle in a box executing 1-d motion, cannot have any value of Energy.

It can have only discrete values of E
 $E = n^2 \Delta$

Note that even Schrödinger equation is for non-relativistic as T operator is $\left(\frac{p^2}{2m} \right)$.



Remember, for H atom, where $\Delta = \left(\frac{h^2}{8mL^2} \right)$

$$2\pi r = n\lambda \quad (n \neq 0)$$

$$p = \frac{h}{\lambda} = \left(\frac{nh}{2\pi r} \right)$$

$$L = p \cdot r = \left(\frac{nh}{2\pi} \right)$$

Bohr Quantization of Ang. Momentum

Quantum (2)

7/02/2012

$$\vec{p} = \hbar \vec{k}$$

$$E = \hbar \omega = mc^2$$

- Canonical Conjugate variables [q, p_x] (position) $x \rightarrow p_x^{(\text{momentum})}$
 (general) $q \rightarrow p_q$
 (lifetime) $t \rightarrow E$ (energy)
 $\theta \rightarrow J$
- Fourier transform expansion coefficient

$$F(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(k) e^{jkx} dk$$

1-d description

Note that it represents superposition of different monochromatic waves, hence it represents a wave group

| | | |
|---------|-------------------------|----------------------|
| diff | $\frac{1}{\sqrt{2\pi}}$ | $\rightarrow \omega$ |
| absolut | x | $\rightarrow p$ |

$$F(x) = \frac{1}{\sqrt{2\pi}} \sum_{k=-\infty}^{\infty} f(k) e^{jkx} \Delta k_x$$

- Moving Particle is equivalent to a moving wave group, which is described by Fourier transform

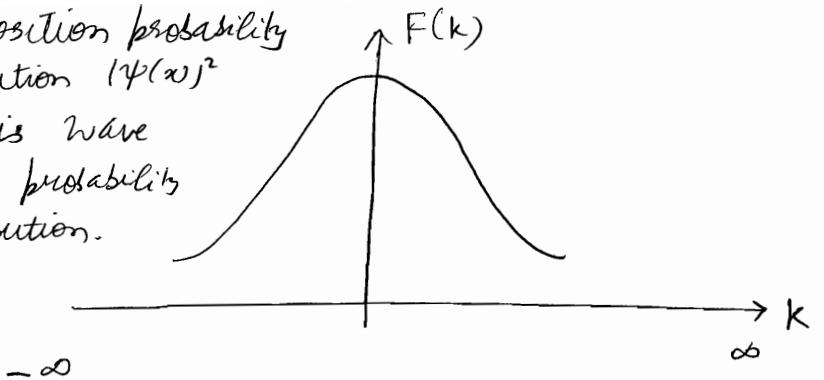
$$\psi(x) = F(x) = \frac{1}{\sqrt{2\pi}} \int f(k) e^{ikx} dk_x$$

Ref eqn. 4.5, 4.6
of H.C. Verma

$$(p = k\hbar)$$

$$\psi(x) = \frac{1}{\sqrt{2\pi\hbar}} \int f(p) e^{\frac{ipx}{\hbar}} dp_x$$

- ② like position probability distribution $|\psi(x)|^2$
 $(f(k))^2$ is wave number probability distribution.



An example of
F(k)

$$f(k) = \frac{1}{\sqrt{2\pi}} \int F(x) e^{-ikx} dx$$

inverse fourier transform

Expansion

Coefficient of moving particle

Fourier transforms of

$x \leftrightarrow k \propto \text{no. } \sqrt{\hbar}$

$p \leftrightarrow k \propto \frac{1}{\sqrt{\hbar}}$ in denominator
for proper units

$$\psi_{(x)} = \psi(x, y, z) = \frac{1}{(2\pi)^{3/2}} \int f(k) e^{i \vec{k} \cdot \vec{x}} d^3 k$$

3-d description

Gaussian Wave Packet Treatment of free particle

Free Particle: No Potential i.e. No external force
hence no restriction at all.

P-65
Verma

$$E_{\text{Total}} = E_{\text{kinetic}} = \frac{p^2}{2m} = \frac{\hbar^2 k^2}{2m}$$

$$\Rightarrow E = E(k) = \left(\frac{\hbar^2}{2m}\right) k^2$$

Now if k is distributed normally,

$$f(k) = A e^{-\left(\frac{k^2}{2\sigma^2}\right)} \quad \text{--- (1)}$$

σ : standard deviation

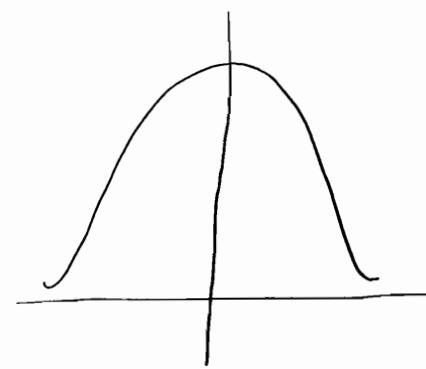
[in general $f(x) = A e^{-\frac{(x-x_0)^2}{2\sigma^2}}$: gaussian distn]

$$\sigma^2 = \text{Mean} [(x-\bar{x})^2]$$

$$= \text{Mean} [x^2 + \bar{x}^2 - 2x\bar{x}]$$

$$= \langle x^2 \rangle + \bar{x}^2 - 2\bar{x}\langle x \rangle$$

$$= \langle x^2 \rangle - \bar{x}^2$$



$$\bar{x} = 0$$

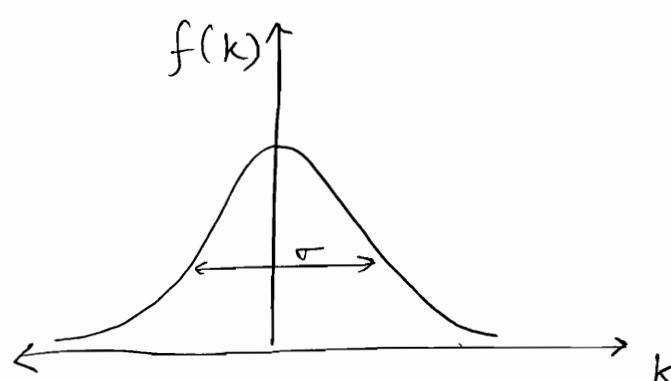
$\sigma = \text{S.D. is error in measurement}$
of x

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

$\langle x \rangle$: Expectation Value of x = $\frac{\sum x f(x)}{\sum f(x)}$

$$\int_{-\infty}^{\infty} f(x) dx = 1$$

$\langle x^2 \rangle$: $\frac{\sum x^2 f(x) dx}{\sum f(x) dx}$



$$\langle k \rangle = \frac{\int_{-\infty}^{\infty} k f(k) dk}{\int_{-\infty}^{\infty} f(k) dk}$$

$$= \Theta$$

$\sigma = \Delta k$: Error in measurement of k .

Given $f(k) = A e^{-\frac{k^2}{2\sigma^2}}$

Finding A s.t. $\int_{-\infty}^{\infty} f(k) dk = 1$ is called Normalization

$$A \int_{-\infty}^{\infty} e^{-\frac{k^2}{2\sigma^2}} dk = 1$$

$$\left[\int_0^{\infty} e^{-x} x^n dx = \sqrt{n+1} \right] \checkmark$$

$$\int_0^{\infty} x^n e^{-\alpha x^2} dx = \frac{1}{2(\alpha)^{\frac{n+1}{2}}} \cdot \sqrt{\frac{n+1}{2}} \quad \begin{matrix} \checkmark \\ \alpha > 0 \\ n > -1 \end{matrix}$$

$$\int_{-\infty}^{\infty} e^{-\alpha x^2 + jkx} dx = \sqrt{\frac{\pi}{\alpha}} e^{\frac{k^2}{4\alpha}} \quad (\alpha > 0) \checkmark$$

$$\Rightarrow A \sqrt{\frac{\pi}{\alpha}} \frac{2\sigma^2}{1} = 1$$

$$\Rightarrow A = \frac{1}{\sqrt{2\pi} \sigma}$$

$$F(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(k) e^{jkx} dk \quad \text{④ Fourier Transform of Gaussian is a Gaussian Function}$$

$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{1}{\sigma \sqrt{2\pi}} e^{-\frac{k^2}{2\sigma^2} + jkx} dk$$

$$= \frac{1}{\sigma \sqrt{2\pi}} \sqrt{\frac{\pi}{(2\sigma^2)}} e^{-\frac{x^2}{4} \cdot \frac{1}{1}} = \frac{1}{\sqrt{2\pi}} e^{-\frac{2\sigma x^2}{2}}$$

Gamma Function

$$\Gamma(n+1) = n \Gamma(n)$$

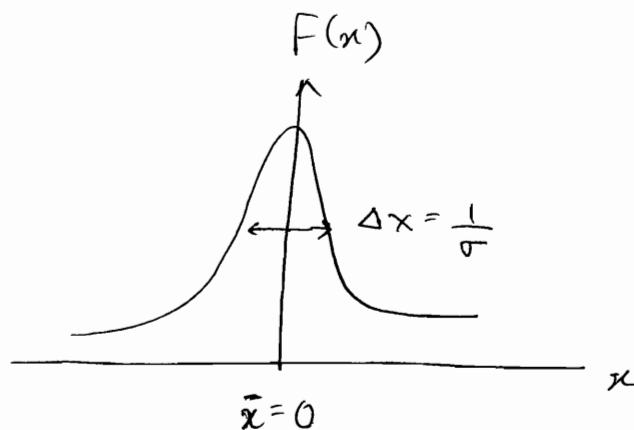
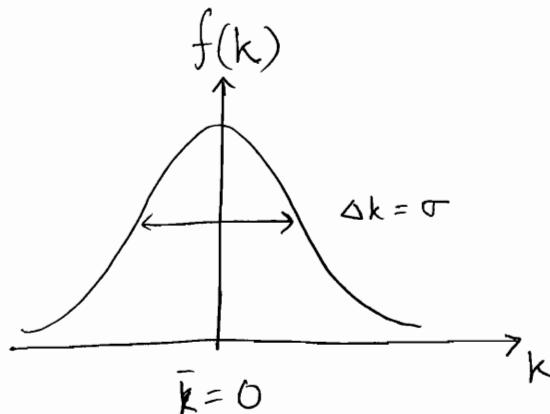
$$\Gamma(1) = 1$$

$$\Gamma(\frac{1}{2}) = \sqrt{\pi}$$

$$\Gamma(n+1) = n \Gamma(n)$$

$$F(k) = \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2(\frac{1}{\sigma})^2}}$$

which turns out to be gaussian distn.



$$\Delta k = \sigma$$

$$\Delta x = \frac{1}{\sigma}$$

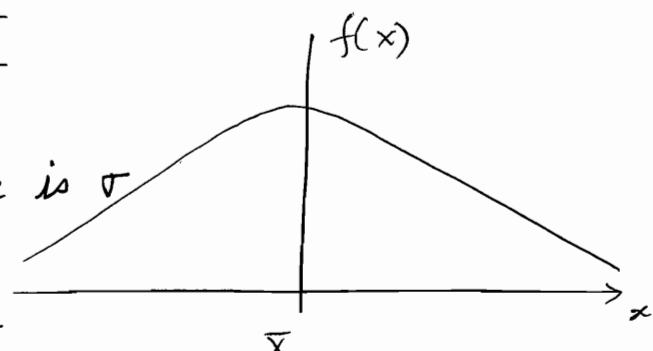
→ Note that Δk can be considered as error in measurement of k or the actual variation of k .

$$\Rightarrow \boxed{\Delta k * \Delta x = 1}$$

$$\Rightarrow \boxed{\Delta x * \Delta p = \hbar}$$

We can start from $f(x) = \text{gaussian}$ and reach the result.

$$f(x) = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(x-\bar{x})^2}{2\sigma^2}}$$



To Prove S.D. of normal curve is σ
let $\bar{x} = 0$

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

$$\sigma^2 = \int_{-\infty}^{\infty} x^2 \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{x^2}{2\sigma^2}} dx = \frac{1}{\sigma\sqrt{2\pi}} \frac{2x}{2\left(\frac{1}{2\sigma^2}\right)^{3/2}} \cdot \frac{\sigma^{3/2}}{2} = \frac{1}{\sqrt{2\pi}\sigma} \cdot \frac{(2\sigma^2)^{3/2}}{2} \cdot \frac{1}{2} \sqrt{\pi}$$

$$= \sigma^2$$

$$= \frac{1}{\sqrt{2\pi}\sigma} \cdot \frac{(2\sigma^2)^{3/2}}{2} \cdot \frac{1}{2} \sqrt{\pi}$$

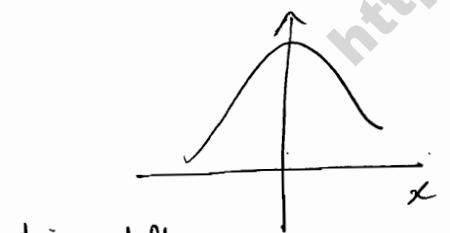
$$\begin{aligned}
 f(k) &= \frac{1}{\sqrt{2\pi}} \int f(x) e^{-ikx} dx \\
 &= \frac{1}{\sqrt{2\pi}} \int \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{x^2}{2\sigma^2} - ikx} dx \\
 &= \frac{1}{\sigma(2\pi)} \sqrt{\frac{\pi}{2\sigma^2}} e^{-\frac{k^2}{4} - \frac{2k^2}{\sigma^2}} \\
 &= \frac{1}{\sqrt{2\pi}} e^{-\frac{k^2}{2(\frac{1}{\sigma})^2}}
 \end{aligned}$$

$$\Rightarrow \Delta x = \sigma$$

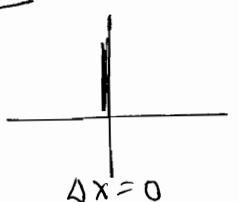
$$\Delta k = \frac{1}{\sigma}$$

$$\Rightarrow \Delta x * \Delta k = 1$$

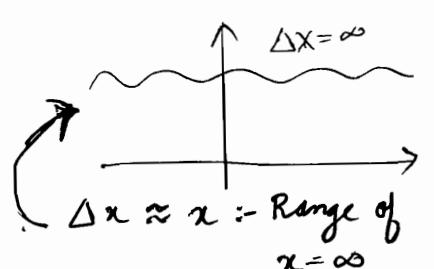
Canonical Conjugate Variables



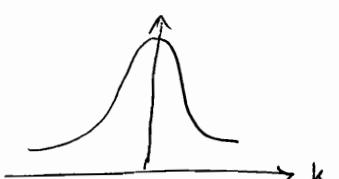
dear delta



$$\Delta x = 0$$

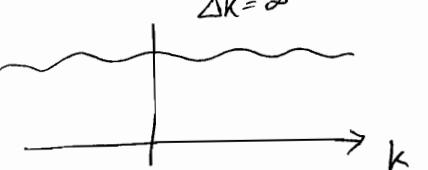


$$\Delta x \approx x - Range of x = \infty$$



$$\Delta x \Delta y = \text{Const.}$$

\uparrow
Both cannot be precisely measured simultaneously



$$\Delta k = \infty$$



plane wave

$$\Delta k = 0$$

$$\Delta k \approx k : \text{Range of } k = \infty$$

$$\Psi(x) = \frac{1}{\sqrt{2\pi}} \int F(k) e^{ikx} dk$$

$$\Psi(x, t) = \left[\frac{1}{\sqrt{2\pi}} \int F(k) e^{ikx} dk \right] [T(t)]$$

$$= \Psi(x) e^{-iwt}$$

$$= \Psi_0 e^{ikx} e^{-iwt}$$

$$= \Psi_0 e^{i(kx - wt)}$$

Since we always take $e^{-iwt} \Rightarrow e^{ikx}$ means wave travelling in positive x direction & $e^{-ikx} \Rightarrow$ negative x dir"

Heisenberg's Uncertainty Principle

Product of errors of 2 conjugate variables's measurement:

$$\Delta q * \Delta p_q \geq \left(\frac{\hbar}{2} \right)$$

Comparing the orders,

$$\Delta q * \Delta p_q \approx \cancel{\hbar} \approx \hbar \approx 10^{-34}$$

$$\boxed{\Delta x \Delta p_x \geq \left(\frac{\hbar}{2} \right)}$$

$$\Delta E \Delta t \geq \left(\frac{\hbar}{2} \right)$$

$$\Delta J \Delta \theta \geq \left(\frac{\hbar}{2} \right)$$

basic Heisenberg relationship

energetic $\vec{J} \vec{J}$ $\vec{\theta} \vec{\theta}$ $\vec{p} \vec{p}$!!

important in

angular momentum quantization
i.e. whole of atomic & nuclear Physics.

$$\textcircled{1} \quad \Delta q \Delta p_q \geq \frac{\hbar}{2}$$

where

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

$$\& \quad \Delta p_q = \sqrt{\langle p_q^2 \rangle - \langle p_q \rangle^2}$$

s.t.

$$\langle q \rangle = \frac{\int q f(q) dq}{\int f(q) dq}$$

$$\langle q^2 \rangle = \frac{\int q^2 f(q) dq}{\int f(q) dq}$$

Illustrations

- 1) e^- cannot reside inside the nucleus. Prove
- 2) Find out ground state radius & energy of H atom.
- 3) Find out minimum energy of Harmonic Oscillator i.e. Parabolic Potential Well.
- 4) Mass of π meson is what, when range of interaction is r ?
(exchange particle)
- 5) Spectral width of any line i.e. $\Delta \nu$.

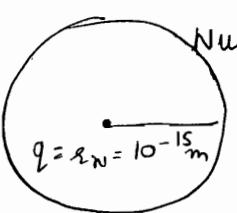
e^- Cannot reside in the nucleus.

take $\left(\frac{\hbar}{2}\right)$

Order of Nuclear Potential Well \approx

$28 - 35$ Mev

If $energy_{e^-} > 35$ MeV \Rightarrow it will escape out.



Nucleus

$$r = r_N = 10^{-15} \text{ m}$$

$$\begin{aligned} \Delta q_{\max} &= 10^{-15} \text{ m} \\ \text{Position} \rightarrow \Delta p_q &\geq \left(\frac{\hbar}{2 \Delta q} \right) \\ \text{Momentum} \end{aligned}$$

$$\Rightarrow \Delta p_x \geq \frac{10^{-34}}{2 \cdot 10^{-15}} = 10^{-19}$$

Momentum must be comparable with error in momentum

$$\Rightarrow p_x \approx 10^{-19}$$

(note that it is
relativistic energy)

$$E = \sqrt{(pc)^2 + (m_0 c^2)^2} \approx pc$$

$[100 > 0.5]$

$$= \frac{10^{-19} \times 3 \times 10^8}{1.6 \times 10^{-13}} \text{ MeV}$$

$$= 100 \text{ MeV}$$

$$\frac{6.6 \times 3 \times 10^8}{2 \times 2\pi \times 1.6} = 0.98 \text{ MeV}$$

We can even put all the values

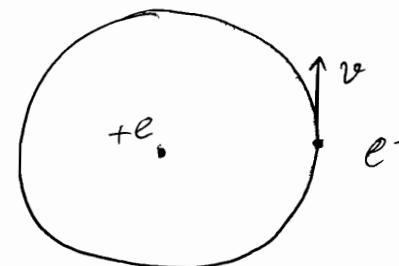
$\Rightarrow E_{e^-}$ if residing in nucleus $= 100 \text{ MeV} > 35 \text{ MeV}$ which is the maximum attractive energy of nucleus.

H atom

take (\hbar)

At r

$$E(r) = \frac{k_e}{2r} - \frac{e^2}{4\pi\epsilon_0 r}$$



We know $\Delta x \Delta p_x \geq \left(\frac{\hbar}{2}\right)$

For minimum energy, $\boxed{\Delta x \Delta p_x \approx \hbar}$

$$\Delta x = x$$

$$\Delta p_x \approx \left(\frac{\hbar}{x}\right) = p_x$$

$$E(r) = \frac{\frac{h^2}{2m} - \frac{e^2}{4\pi\epsilon_0 r}}{r}$$

Note that

$$m = m_e$$

For ground state

$$\left. \frac{dE}{dx} \right|_{x=r_0} = 0, \quad \left. \frac{d^2E}{dx^2} \right|_{x=r_0} > 0$$

As atom is assumed to be at rest

(*) do not use approximations like $r^2 = 10$ or $\frac{h}{r} = 10^{-34}$ as the values are too small s.t. approximation completely changes the answer!!

kE is possessed by e^- only.

$$\left[\frac{4\pi\epsilon_0 h^2}{me^2} \right]$$

$$r_0 = 0.53 \text{ \AA}$$

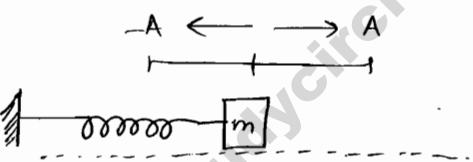
$$-\frac{me^4}{32\pi^2\epsilon^2 h^2}$$

$$E_{g0} = -13.6 \text{ eV}$$

(*) do not forget $\frac{1}{2\pi}$ in expression of k

Simple Harmonic Oscillator : Minimum Energy

take $\left(\frac{k}{2}\right)$
and $2\pi = \Delta t = \left(\frac{k}{2}\right)^{-1}$



refer Verma : P-67

$$V = \frac{1}{2} kx^2$$

$$E = \frac{p_x^2}{2m} + \frac{1}{2} kx^2$$

just to remember

$$\Delta x \Delta p_x \approx \hbar$$

(we cannot write minimum here
as we have to maximize afterwards)

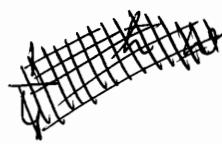
$$\Delta x = 2A$$

$$\Delta p_x = \frac{\hbar}{2A} \approx p_x$$

$$E(A) = \frac{\hbar^2}{8mA^2} + \frac{1}{2} kA^2$$

$$\text{Put } \frac{dE}{dA} = 0 \quad -\frac{2h^2}{8m A^3} + kA = 0 \Rightarrow A = \sqrt[3]{\frac{2h^2}{8mk}}$$

$$\Rightarrow A^2 = \frac{h^2}{2\sqrt{mk}}$$



$$E = \frac{1}{2}\sqrt{k} \frac{\hbar^2}{2\sqrt{m}} + \frac{\hbar^2}{8m} \frac{2\sqrt{mk}}{h}$$

$$= \frac{1}{4} \hbar^2 \sqrt{\frac{k}{m}} + \frac{1}{4} \hbar^2 \sqrt{\frac{k}{m}}$$

$$= \frac{1}{2} \hbar \sqrt{\frac{k}{m}} \Rightarrow E(a) = \frac{1}{2} \hbar \omega$$

Mass of Exchange Particle

$$\Delta E \Delta t \approx \frac{\hbar}{\alpha}$$

$$E = mc^2 \quad mc^2 \frac{R}{c} \approx \frac{\hbar}{\alpha}$$

$$\Delta t = t = \frac{R}{c} \quad \frac{\text{range}}{\text{velocity}} \quad m \approx \left(\frac{\hbar}{RC} \right)$$

Spectral Width

take

$$E = h\nu$$

$$\Delta E \Delta t \approx \frac{\hbar}{\alpha}$$

$$\Delta\nu \Delta t \approx 1 \Rightarrow \underline{\Delta\nu = \frac{1}{\Delta t}}$$

Proof of Heisenberg

Step 1 Given X and P_x are two conjugate variables.

Define $X' = X - \langle X \rangle$
 $P'_x = P_x - \langle P_x \rangle$

Step 2

Now $(\Delta X)^2 = \langle X^2 \rangle - \langle X \rangle^2$
 $= \langle X'^2 \rangle \quad \dots \quad (1)$

$$(\Delta P_x)^2 = \langle P_x^2 \rangle - \langle P_x \rangle^2
= \langle P_x'^2 \rangle \quad \dots \quad (2)$$

Also $[X', P_x']$

$$= [X - \langle X \rangle, P_x - \langle P_x \rangle]
= [X, P_x] \quad \dots \quad (3)$$

Step 3

Let us consider an arbitrary state $|\psi\rangle$, an arbitrary real number λ and construct a state $|\phi\rangle$ s.t.

$$|\phi\rangle = (X' + i\lambda P') |\psi\rangle$$

Step 4

We know $\langle \phi | \phi \rangle \geq 0$ for any λ and $|\psi\rangle$

$$\Rightarrow \langle \psi | X'^2 | \psi \rangle - i\lambda \langle \psi | P' X' | \psi \rangle + i\lambda^2 \langle \psi | X' P' | \psi \rangle + \lambda^2 \langle \psi | P'^2 | \psi \rangle \geq 0$$

(do not worry about P'^2
and we can write $i\hbar \frac{d}{dx}$ as iP)

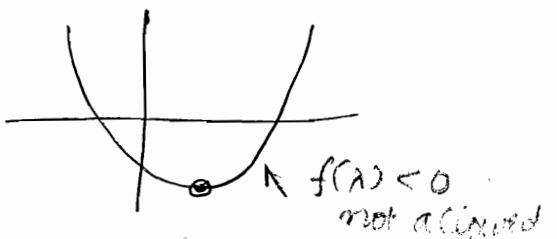
$$\Rightarrow \lambda^2 \langle P'^2 \rangle + \lambda \langle i[X', P] \rangle + \langle X'^2 \rangle \geq 0$$

Using (1), (2), (3)

$$\Rightarrow (\Delta p)^2 \lambda^2 + \langle i[X, P] \rangle \lambda + (\Delta x)^2 \geq 0$$

Step 5

It's a parabola in λ with $a > 0$



$$f(\lambda) = a\lambda^2 + b\lambda + c$$

$$\text{Minima} @ \lambda_{\min} = -\frac{b}{2a}$$

$$\text{Minimum value} = c - \frac{b^2}{4a}$$

$$\therefore f(\lambda) \geq 0$$

$$\Rightarrow c - \frac{b^2}{4a} \geq 0$$

$$\Rightarrow ac \geq \frac{b^2}{4}$$

Hence

$$(\Delta x)^2 (\Delta p_x)^2 \geq \frac{\langle i[X, P] \rangle^2}{4}$$

Step 6

$$\text{Put } [X, P] = i\hbar$$

$$\Rightarrow \boxed{\Delta x \Delta p_x \geq \frac{\hbar}{2}}$$

$$(in \text{ general } \Delta a \Delta b \geq \frac{\langle [A, B] \rangle}{4})$$

Quantum (3)

08/02/12

Mathematical Proof of Heisenberg's Principle.

From Schwartz Inequality,

$$\int f^* f \, d\tau \int g^* g \, d\tau \geq \frac{1}{4} \int |(f^* g + g^* f)^2| \, d\tau$$

$$\langle x \rangle = 0 \quad \langle p_x \rangle = 0$$

Let us take

$$f = P_x \psi = -i\hbar \left(\frac{\partial \psi}{\partial x} \right)$$

$$g = ix\psi$$

Evaluating the 1^{st} term of LHS

$$\begin{aligned} \int f^* f \, d\tau &= \int_V \left(i\hbar \frac{\partial \psi^*}{\partial x} \right) \left(-i\hbar \frac{\partial \psi}{\partial x} \right) \, d\tau \\ &= \hbar^2 \int_V \frac{\partial \psi^*}{\partial x} \frac{\partial \psi}{\partial x} \, d\tau \end{aligned}$$

$$= \hbar^2 \iiint \begin{matrix} \text{I} \\ \left(\frac{\partial \psi}{\partial x} \right) \end{matrix} \begin{matrix} \text{II} \\ \left(\frac{\partial \psi^*}{\partial x} \right) \end{matrix} dx dy dz$$

Integrating w.r.t. x, (Integration by parts)

$$= \hbar^2 \iiint \left[\left(\frac{\partial \psi}{\partial x} \right) \psi^* \right]_{-\infty}^{\infty} dy dz - \hbar^2 \iiint \left(\frac{\partial^2 \psi}{\partial x^2} \right) \psi^* dx dy dz$$

$\underbrace{\hspace{10em}}$

$$= 0$$

$$= -\hbar^2 \int_V \left(\frac{\partial^2 \psi}{\partial x^2} \right) \psi^* dx dy dz$$

$$= \int_V \psi^* \left(-\hbar^2 \frac{\partial^2}{\partial x^2} \right) \psi d\tau$$

$$= \int_V \psi^* P_x^2 \psi d\tau$$

$$= \langle p_x^2 \rangle$$

$$\boxed{(\Delta p_x)^2 = \langle p_x^2 \rangle - \langle p_x \rangle^2 \therefore = \langle p_x^2 \rangle}$$

$$= (\Delta p_x)^2 \quad (\text{i.e. } \sigma_p^2)$$

$$g = ix\psi \quad g^* = -ix\psi^*$$

$$\begin{aligned} & \int g^* g d\tau \\ &= \int -ix\psi^* ix\psi d\tau \\ &= \int \psi^* \psi x^2 d\tau \\ &= \langle x^2 \rangle = (\Delta x)^2 \quad (\text{i.e. } \sigma_x^2) \end{aligned}$$

We have taken

$$\int f^* f d\tau \quad \int g^* g d\tau \geq \frac{1}{4} \int |f^* g + g^* f| d\tau$$

$$f = P_x \psi = -i\hbar \frac{\partial \psi}{\partial x}$$

$$g = i x \psi = i x \psi$$

$$\text{L.H.S.} = (\Delta p_x)^2 (\Delta x)^2$$

R.H.S

Proof of Heisenberg limit to be Gaussian Function

Wave Function

Till now, we have seen any particle can be described as a wave group. It can be represented as

$$\psi(x, t) = \psi(x) T(t)$$

$$T(t) = e^{-i\omega t}$$

$$\psi(x) = \psi(x, y, z) = \frac{1}{(\sqrt{2\pi})^3} \iiint F(k) e^{i\vec{k} \cdot \vec{x}} d^3k$$

since $\psi(x) = \frac{1}{\sqrt{2\pi}} \int F(k) e^{i k \cdot x} dk$

$$\Rightarrow \psi(x) = A(k) e^{ikx}$$

Also, k and ω are canonical conjugates i.e. both cannot be determined precisely simultaneously.

hence

$$\psi(x, t) = A(k) e^{i(kx - \omega t)}$$

Wave Function In this eqn, inbuilt are

- ① Planck's Quantization
- ② De Broglie's wave theory

Note that Wave Function is not displacement Heisenberg Uncertainty Principle

It is the state representation of quantum behaviour of particle i.e. complete description or representation of its state.

Axioms of Quantum Mechanics

① Concept of Wave Function

$\psi(x, t)$: Complete representation of 'state'

② Max Born's Explanation of ψ

(Probability density of locating a particle in some region) $\propto |\psi|^2$

Prob. density $\propto |\psi|^2 \propto \psi^* \psi$

$$\frac{dP}{dT} \propto \psi^* \psi$$

$$\Rightarrow dP \propto \psi^* \psi dT$$

Probability $\propto \int_V \psi^* \psi d\tau$ ← Hence $\psi(x)$ has units of $\frac{1}{\sqrt{\text{Length}}}$
 and $\psi(r)$ has units of $\frac{1}{\sqrt{\text{Volume}}}$, no part $\sqrt{\text{Volume}}$
 e^{ikx} in calculation of Probability. $[e^{ikx} * e^{-ikx} = 1]$

$$\boxed{\text{Prob} \propto \int_V \psi^*(x) \psi(x) d\tau} \quad 3-d$$

$$\boxed{\text{Prob} \propto \int \psi^*(x) \psi(x) dx} \quad 1-d$$

$$d\tau = dx dy dz$$

$$d\tau = r^2 \sin\theta dr d\theta d\phi$$

$$= 4\pi r^2 dr \quad (\text{if independent of } \theta, \phi)$$

Orthogonal
norm = 1

Orthonormality Condition on Wave Function

$$\int_V \psi_m^* \psi_n d\tau = \delta_{mn}$$

; Kronecker Delta Function

$= 1 \quad \text{if } m=n$
 $= 0 \quad \text{if } m \neq n$

Total space

$$\int_V \psi_1^* \psi_2 d\tau = 0$$

$$\int_V \psi_1^* \psi_1 d\tau = 1$$

- It also states that simultaneously, particle cannot be found in 2 states m and n .

③ Wave Function must be well behaved.
i.e. single valued, finite and continuous

↑
normal
"function"

↑
square
integrable

and derivative
should be
continuous as well

FINITE

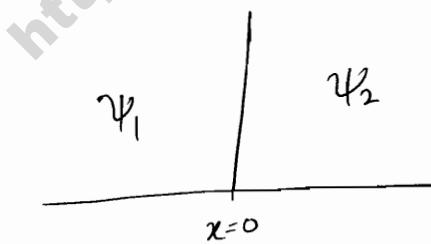
$\psi = e^{kx}$: Not possible as $\psi \rightarrow \infty$
as $x \rightarrow \infty$

Good Function for $x < 0$

$\psi = \tan x$: Not possible as $\psi \rightarrow \infty$
as $x \rightarrow (\pi/2)$

$\psi = \sin x$: good function

CONTINUOUS



$$\lim_{x \rightarrow 0^-} \psi_1 = \lim_{x \rightarrow 0^+} \psi_2$$

~~if differentiable~~
$$\left(\frac{d\psi_1}{dx} \right) = \left(\frac{d\psi_2}{dx} \right)$$
 ~~if continuous~~

if $\Delta V \neq \infty$

④ Along with every physically observable quantity, quantum mechanics associates Mathematical Operators.

This axiom is related to measurement of physical quantities.

Physically Observable Quantity
(small)

"Hermitian" Operator
(capital)

① Position \vec{r}

 \vec{r}

② Momentum
linear

 \vec{p}
 $-i\hbar \vec{\nabla}$
 p_x
 $-i\hbar \frac{\partial}{\partial x}$
 p_y
 $-i\hbar \frac{\partial}{\partial y}$
 p_z
 $-i\hbar \frac{\partial}{\partial z}$

③ Momentum
Angular

$$\vec{J} = \vec{r} \times \vec{p}$$

$$= -i\hbar (\vec{r} \times \vec{\nabla})$$

④ Energy "E"

$$i\hbar \frac{\partial}{\partial t}$$

○ Remember from EM

$$\vec{\nabla} \equiv i\vec{k}$$

$$-i\vec{\nabla} = \vec{k} = \frac{\vec{p}}{\hbar} \Rightarrow \underline{\underline{\vec{p}}} = -i\hbar\vec{\nabla}$$

$$\frac{\partial}{\partial t} \equiv -i\omega$$

$$+i\frac{\partial}{\partial t} = \frac{E}{\hbar k} \Rightarrow E = \underline{\underline{+i\hbar\frac{\partial}{\partial t}}}$$

⑤ kinetic Energy

$$T = \frac{\vec{p}^2}{2m} \quad -\frac{\hbar^2}{2m}\nabla^2$$

⑥ Potential Energy

$$V \quad V$$

⑦ Mechanical
Energy

$$T+V$$

H (Hamiltonian)

$$= T+V$$

$$= -\frac{\hbar^2}{2m}\nabla^2 + V$$

○ Hermitian Operator A if $\int_{\tau} \psi_1^* [A \psi_2] d\tau$

$$= \int [A\psi_1]^* \psi_2 d\tau$$

i.e. $\langle A\psi_1 | \psi_2 \rangle = \langle \psi_1 | A\psi_2 \rangle$ i.e. Operator can be linked with any wave function
Hermitian Operator will give only real values.

⑤ Eigen Value Problem

(Most important)

$$a\psi = A\psi$$

Any dynamical variable 'a' can only assume only those value which are solutions of Eigen Value Problem.

GIST OF QUANTUM THEORY
Since every dynamical variable is quantized i.e. can have only definite values or not a continuous

$A \Psi_n = a_n \Psi_n$

↑

Mathematical a_n : eigen values
operator Ψ_n : states or eigen functions

$$A \Psi_1 = a_1 \Psi_1 \quad \text{Prob} = |\Psi_1|^2$$

$$A \Psi_2 = a_2 \Psi_2$$

:

$$A \Psi_n = a_n \Psi_n$$

We also write,

$$A |\Psi\rangle = a |\Psi\rangle$$

We had studied in matrices,

$$A X = \lambda X$$

↑
eigen values

eigen functions / vectors

Example

: ① Measure Momentum p_x ,

$$p_x \Psi = -i\hbar \frac{\partial}{\partial x} \Psi$$

② Measure position x ,

$$x \Psi = x_0 \Psi$$

$$\Rightarrow \Psi = \underline{\delta(x-x_0)}$$

[Dirac Delta]

$$\Rightarrow \frac{d\Psi}{\Psi} = -\frac{p_x}{i\hbar} dx = \frac{i}{\hbar} p_x dx$$

$$\Rightarrow \ln \Psi = \frac{i p_x}{\hbar} x + \underline{\ln A}$$

$$\Rightarrow \Psi = A e^{i \frac{p_x x}{\hbar}}$$

[Plane wave]

Now ψ cannot be imaginary, otherwise ψ can become ∞
 anyways, ψ cannot be a eigenfunction of course. as its not square integrable. It can be wavefunctions

② Measure Energy

$$H\psi_n = E_n \psi_n$$

$$H\psi = \left(\frac{p^2}{2m} + V \right) \psi = E\psi \quad (\text{LHS}) \quad (\text{RHS})$$

Schrödinger's Wave Equation :

$$\left(-\frac{\hbar^2}{2m} \nabla^2 + V \right) \psi = E\psi$$

Time independent form

$$\text{Put } E(\psi) = i\hbar \left(\frac{\partial \psi}{\partial t} \right) \rightarrow \text{Time dependent form}$$

$$\text{i.e. } -\frac{\hbar^2}{2m} \nabla^2 \psi + V\psi = i\hbar \left(\frac{\partial \psi}{\partial t} \right)$$

③ Angular Momentum :-

$$L^2 \psi = \lambda \psi$$

Operator (Eigen Function) = (Eigen values) (Eigen Functions)

$$|\psi\rangle = \{ \psi_1, \psi_2, \psi_3, \dots, \psi_n \}$$

$$a_n = \{ a_1, a_2, \dots, a_n \}$$

⑥ Expectation Value or Most representative Value

$$\langle a \rangle = \frac{\sum_n \psi_n^* A \psi_n}{\sum_n \psi_n^* \psi_n}$$

Note that it is discrete

$$\langle \psi | A | \psi \rangle = \frac{\int \psi^* A \psi d\tau}{\int \psi^* \psi d\tau}$$

if it is

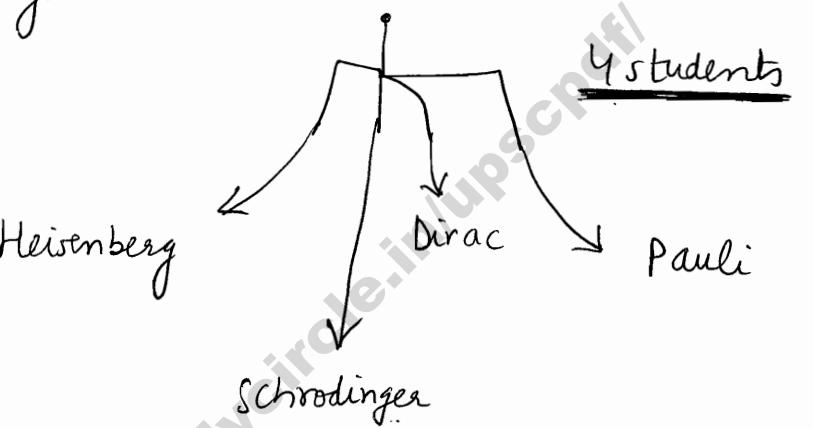
continuous

use of this defⁿ eliminates random constants associated with ψ due to normalization & $\int \psi^* \psi d\tau = 1$ simplifies calculations

If Normalized Wave Function, then $\int \psi^* \psi d\tau = 1$

1926 - 1930

Copenhagen : Niels Bohr



Representation of A in Matrix Form : Heisenberg's description

$$A = \text{Matrix Form} \\ = A [I]_n$$

$$H_{mn} = \langle \psi_m | H | \psi_n \rangle$$

$$\begin{vmatrix} \langle \psi_1 | H | \psi_1 \rangle & \langle \psi_1 | H | \psi_2 \rangle & \dots \\ \vdots & \ddots & \\ \langle \psi_n | H | \psi_1 \rangle & \dots & \langle \psi_n | H | \psi_n \rangle \end{vmatrix}$$

Representation in Bra-ket Form : Dirac's description
BRA KET

$$\langle \psi | A | \psi \rangle = \int \psi^* A \psi d\tau$$

$\langle |$: Bra : ψ^*
 $| \rangle$: ket : ψ

$$(\langle \cdot | \cdot \rangle)^* = |\cdot \rangle$$

$$\langle m | n \rangle = \delta_{mn}$$

$$\langle a \rangle = \langle \psi | A | \psi \rangle = \langle n | A | n \rangle$$

\uparrow
 n^{th} state

Quantum Physics (4)

09/02/12

We have learnt already

✓ For dynamical operator a , we have Operator A
 A can be in form of matrix.

- ⇒ Addition, Multiplication of Operators like Matrices
- ⇒ $AB \neq BA$

✓ Eigen Value Problem

$$A \psi_n = a_n \psi_n$$

where $\{|\psi\rangle\}$ Eigen states or Eigen Functions

These 2 are
solutions of
the above eqn!!

$\{a_n\}$ Eigen values of variable a

✓ Expectation value of ' a ' i.e. [Most representative value among $\{a_n\}$]

$$\langle a \rangle = \langle \psi | A \psi \rangle = \int \psi^* A \psi \, dx$$

if ψ is normalized function divide $\int \psi^* \psi \, dx$!!

$$\underbrace{\frac{a}{\hbar} \psi}_{\text{operator}} = \underbrace{-i\hbar \frac{\partial}{\partial x} \psi}_{\text{operator}}$$

Momentum

$$\Rightarrow \psi = A e^{i \frac{\hbar p_x x}{\hbar}} \quad [\text{Trigonometric}]$$

$$\underbrace{T \psi}_{\text{operator}} = \underbrace{-\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2}}_{\text{operator}} \quad \underline{\text{kinetic Energy}}$$

$$\frac{d^2 \psi}{dx^2} + \left(\frac{2mT}{\hbar^2} \right) \psi = 0$$

This is 2nd order differential equation.

$$\text{Put } \frac{d}{dx} = D \quad \frac{d^2}{dx^2} = D^2 \quad k^2 = \frac{2mT}{\hbar^2}$$

$$(D^2 + k^2) \psi = 0$$

Solution :- $\psi_x = A e^{ikx} + B e^{-ikx}$ [Trigonometric solution]
 $= C_1 \sin kx + C_2 \cos kx$

Solution of $(D^2 - k^2)\psi = 0$: [exponential solution]

Big Bracket []

Big Bracket [] in Quantum Physics is Commutator

$$[A, B] = AB - BA$$

(where A & B are operators)

A and B are said to commute if $[A, B] = 0$

$$\text{i.e. } AB = BA$$

If A and B are commutative i.e. $AB = BA$

\Rightarrow 'a' and 'b' variables are simultaneously measurable

\Rightarrow they are satisfied by same eigenfunctions.

(Somewhat
similar to
Kronecker Delta
Function)

To measure 'a' in state $\psi \Rightarrow A\psi = a\psi \quad \text{--- (1)}$

and also measure 'b' in same state $\psi \Rightarrow B\psi = b\psi \quad \text{--- (2)}$

Premultiply (1) by B and (2) by A

$$B(A\psi) = B(a\psi)$$

$$BA\psi \neq B a\psi = a B\psi = ab\psi \quad - \textcircled{1}$$

$$A(B\psi) = A(b\psi)$$

$$\Rightarrow AB\psi = A b\psi = b A\psi = ab\psi \quad - \textcircled{2}$$

$$\textcircled{2} - \textcircled{1}$$

$$AB\psi - BA\psi = 0$$

$$\Rightarrow (AB - BA)\psi = 0$$

$$\Rightarrow [A, B]\psi = 0$$

Eg.

$$[px, \frac{p^2}{2m}] = 0$$

$$\frac{1}{2m} [px, p^2] = 0$$

(units : per second)

* Operation ψ is
normal \vec{t} , \vec{t}^*
conjugate \vec{t}^* !!

Probability Current Density

No. of particles crossing through a given section per unit time

$$J_x = \frac{\hbar}{2mi} \left[\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x} \right]$$

Refer
Ch - 11

$$\vec{J} = \frac{\hbar}{2m i} [\psi^* \vec{\nabla} \psi - \psi \vec{\nabla} \psi^*]$$

(crossing)
or
(transmitted)

It is fraction of particles (scattered)/(incident)
per unit time.

Wave

\Leftrightarrow

EM

\Leftrightarrow

Quantum

Intensity

Poynting Vector

Prob. Current Density

Same thing
in various subjects...

From Continuity Condition,

$$\vec{\nabla} \cdot \vec{J} + \left(\frac{\partial \rho}{\partial t} \right) = 0$$

Current
density

charge
density

[valid for conservation
of charge / mass]

- Note that in quantum physics, I am not interested in time derivative

In 1-d,

$$\frac{d J_x}{dx} + \frac{d \rho}{dt} = 0$$



ρ: Probability density = $\psi^* \psi$

$$\Rightarrow \frac{d J_x}{dx} = - \frac{\partial \rho}{\partial t} = - \left[\psi^* \frac{\partial \psi}{\partial t} + \psi \frac{\partial \psi^*}{\partial t} \right]$$

We will calculate time derivative of ψ and ψ^* from Hamiltonian

We know $H\psi = E\psi$

$$\left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V \right) \psi = i\hbar \frac{\partial}{\partial t} \psi$$

$$\Rightarrow \frac{\partial \psi}{\partial t} = \frac{1}{i\hbar} \left(-\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V \right) \psi$$

Complex Conjugating,

$$\frac{\partial \psi^*}{\partial t} = - \frac{1}{i\hbar} \left(-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} + V^* \right) \psi^*$$



$$\Rightarrow \frac{d J_x}{dx} = - \frac{1}{i\hbar} \left[\psi^* \left\{ -\frac{\hbar^2}{2m} \frac{\partial^2 \psi}{\partial x^2} + V \psi \right\} - \psi \left\{ -\frac{\hbar^2}{2m} \frac{\partial^2 \psi^*}{\partial x^2} + V^* \psi^* \right\} \right]$$

$$= -\frac{1}{i\hbar} \left\{ \frac{-\hbar^2}{2m} \psi^* \frac{\partial^2 \psi}{\partial x^2} + \cancel{V\psi} + \frac{\hbar^2}{2m} \psi \frac{\partial^2 \psi^*}{\partial x^2} - \cancel{V\psi} \right\}$$

* For hermitian operator
 $\psi^* V \psi = \psi V^* \psi^*$

$$= -\frac{1}{i\hbar} \frac{-\hbar^2}{2m} \left\{ \psi^* \frac{\partial^2 \psi}{\partial x^2} - \psi \frac{\partial^2 \psi^*}{\partial x^2} \right\}$$

★ $\rightarrow = \frac{+\hbar}{2mi} \frac{\partial}{\partial x} \left[\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x} \right]$

$$\Rightarrow \frac{\partial J_x}{\partial x} = \frac{\hbar}{2mi} \frac{\partial}{\partial x} \left[\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x} \right]$$

$$\Rightarrow J_x = \frac{\hbar}{2mi} \left[\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x} \right]$$

$A = \frac{d^2}{dx^2}$

$$\psi = \sin nx$$

Find out Eigen Values

$$a \sin nx = \frac{d^2}{dx^2} (\sin nx) = -n^2 \sin nx$$

$$\Rightarrow a = -n^2$$

For state $\sin x$:- eigen value : -1
 For state $\sin 2x$:- eigen value : -4

and so on...

Q31) Tut2

$$\vec{J} = \frac{\hbar}{2mi} \left[e^{-i(kx-\omega t)} e^{i(kx-\omega t)} ik - e^{i(kx-\omega t)} e^{-i(kx-\omega t)} -ik \right]$$

$$g=1 = \frac{\hbar}{2mi} \cdot 2ik = \frac{\hbar k}{m} = \frac{p}{m} = v$$

32

$$H = -\frac{d^2}{dx^2} + x^2$$

$$\psi(x) = Ax e^{-\left(\frac{x^2}{2}\right)}$$

Eigen Function if

$$H\psi = \lambda \psi \quad \text{where } \lambda \text{ can be any number}$$

$$\begin{aligned} & -\frac{d}{dx} \left[A e^{-x^2/2} + Ax^2 e^{-x^2/2} \right] + x^2 \left[Ax e^{-x^2/2} \right] \\ &= 3Ax e^{-x^2/2} = 3\psi \end{aligned} \quad \boxed{\text{Eigen value} = 3}$$

28 $\langle \psi | \psi \rangle = 1$

$$\Rightarrow \int_{-\infty}^{\infty} \psi^* \psi dx = 1 \quad (\text{l-d case})$$

$$= \int_{-\infty}^{\infty} A^2 e^{-4x^2} dx = 1$$

$$= A^2 \sqrt{\frac{\pi}{4}} = 1$$

$$\Rightarrow A = \left(\frac{4}{\pi}\right)^{1/4}$$

$$\psi(x) = \left(\frac{2}{\sqrt{\pi}}\right)^{\frac{1}{2}} e^{-2x^2} \quad \text{Yes ; eigen value} = 4\lambda$$

$$P_x dx = \psi^* \psi dx$$

$$P_x = \int_{-\infty}^{\infty} \psi^* \psi dx = \frac{2}{\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-4x^2} dx$$

$$\text{Put } 4x^2 = y \quad = \frac{2}{\sqrt{\pi}} \int_0^{\infty} e^{-y} dy \quad [\text{even function}]$$

$$= \frac{2}{\sqrt{\pi}} \cdot \frac{1}{2(4)^{\frac{1}{2}}} \sqrt{\frac{1}{2}} = \frac{2}{\sqrt{\pi}} \cdot \frac{1}{4} \sqrt{\frac{1}{2}} = \frac{1}{2} \sqrt{\frac{1}{2}}$$

(iv) Yes

$$\langle \psi_m | \psi_n \rangle = \delta_{mn}$$

$$\int \psi_m^* \psi_n \, dx = 0$$

$$\int x \psi^* \psi \, dx = 0$$

↑
odd function

Hence LHS = 0

$$\int_{-\infty}^{\infty} x e^{-4x^2} \, dx = 0$$

✓ If I know ψ , I know errors of all variables,

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

expectation value of all variables

$$\langle a \rangle \stackrel{v}{=} \langle \psi | A | \psi \rangle$$

✓ Schrodinger Wave Equation is nothing but eigen value problem of energy.

✓ In order to calculate 'most probable' phenomenon, maximize the Probability

Note that it is not expectation value I throw a dice 6 times 5 times 1 1 time 6

$$dP = \psi^* \psi \, 4\pi r^2 \, dr$$

: Maximize $dP \propto P_{\max} = 1$
 $\langle x \rangle = \left(\frac{11}{6}\right)$

✓ All the problems defined in course are time independent.
i.e. stationary state solutions

e.g. e- in 1 state : time independent energy

but if $\begin{cases} \text{e- jumps from 1st to 2nd state : time dependent energy} \\ \text{current in superconductors : time dependent } \frac{dq}{dt} \end{cases}$

$$H \Psi_n = E_n \Psi_n : \text{Schrodinger Wave Eqn}$$

$$\left(-\frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V \right) \psi_n = E_n \psi_n$$

$$\Rightarrow \frac{\hbar^2}{2m} \frac{d^2\psi}{dx^2} + (E_n - V) \psi_n = 0$$

$$\Rightarrow \boxed{\frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2} (E - V) \psi = 0}$$

$$\Rightarrow \boxed{\frac{d^2\psi}{dx^2} + k^2 \psi = 0}$$

the most standard
form of
Schrodinger wave
Equation

$$\text{where } k^2 = \frac{2m}{\hbar^2} (E - V)$$

$$= \frac{b x^2}{\hbar^2} = k^2 = \left(\frac{2\pi}{\lambda}\right)^2$$

Hence this k is the wave number.
(classically)

$$\text{We know, classically } E = T + V$$

$$E - V = T > 0$$

$$\Rightarrow E - V > 0$$

$$\Rightarrow +k^2$$

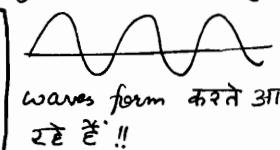
\Rightarrow Trigonometric solution

If anyhow $-k^2$

$$\Rightarrow -k^2$$

\Rightarrow Exponential solution

• जो एम् classically



waves form करते हैं !!

वहाँ type का solution
जो exponentially
decay कर रहे हैं

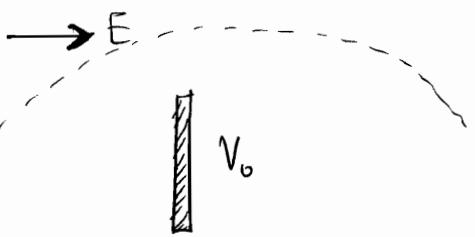
$$\text{if } (E - V) > 0$$

$$\Rightarrow \Psi_{(x)} = A e^{ikx} + B e^{-ikx}$$

$$\xrightarrow{+x} \quad \xleftarrow{-x}$$

: Standing wave :
Confined to a region

V_0 : Potential Barrier



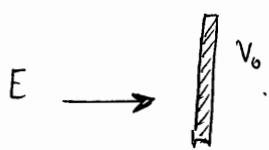
[classically]

① 2 things to note

(i) in Quantum, Potential is same as Potential energy

(ii) Do not think of Potential as something possessed by a particle. A particle only possesses E. Potential is minimum E required to cross a hurdle.

quantum mechanical tunneling



$$\frac{d^2\psi}{dx^2} - \frac{2m}{\hbar^2} [V - E] \psi = 0$$

$$\frac{d^2\psi}{dx^2} - k'^2 \psi = 0$$

$$k'^2 = \frac{2m}{\hbar^2} [V - E]$$

$$\psi_x = A e^{k'x} + B e^{-k'x}$$

$$-\infty < x < 0 : A e^{k'x}$$

$$0 < x < \infty : B e^{-k'x}$$

Problem 1:

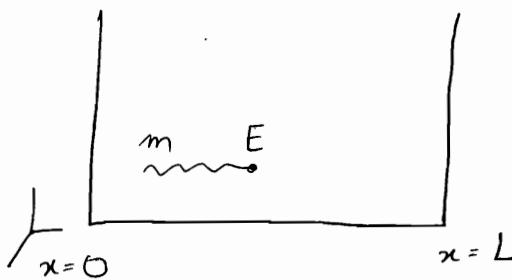
1-d Box (single Particle)
[Infinite Potential Well Problem]

$$\psi(x) = 0 \quad \begin{matrix} \text{at } x=0 \\ \text{at } x=L \end{matrix}$$

$$H(\psi) = E(\psi)$$

$$V=0$$

$$H = \frac{p^2}{2m}$$



$$\Rightarrow \frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2} \psi = 0$$

$$\Rightarrow \frac{d^2\psi}{dx^2} + k^2 \psi = 0$$

$$\Rightarrow \psi_{(x)} = A \sin kx + B \cos kx$$

$$\left. \begin{array}{l} 0 = B \cos 0 \\ 0 = A \sin kL \end{array} \right\} \text{Boundary Conditions}$$

A cannot be 0, otherwise Wave Function will vanish

$$\Rightarrow kL = n\pi \quad n=1, 2, 3, \dots$$

$$\Rightarrow k_n = \frac{n\pi}{L}$$

$$k_n^2 = \frac{2mE}{\hbar^2} = \frac{n^2\pi^2}{L^2}$$

$$\Rightarrow E_n = \boxed{\frac{n^2\hbar^2\pi^2}{2mL^2}} = \left(\frac{n^2\hbar^2}{8mL^2}\right) = n^2 \Delta$$

$$\psi_n(x) = A \sin\left(\frac{n\pi x}{L}\right)$$

Note that solution of eigen ~~value problems~~ are eigen functions and eigen values
 $A\psi = a\psi$

Solution : ψ_n, a_n

Normalizing Wave Function

$$\int A^2 \sin^2 \frac{n\pi x}{L} dx = 1$$

$$A^2 \frac{L}{2} = 1$$

$$\Rightarrow A = \sqrt{\frac{2}{L}}$$

$$\Rightarrow \boxed{\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)}$$
$$E_n = n^2 \left(\frac{\pi^2 h^2}{2m L^2} \right)$$

Final solutions are represented in terms of Quantum Numbers.

① Now comparing it with results derived in lecture 1, we get that:

(1) What we assumed that different loops of stationary waves are nothing but different "eigen functions" or "states" in which particle is found. [n = number of loops]

(2) With the previous assumption, we were able to derive only Energy. But now with precise knowledge of Ψ , we can derive any variable's expectation value.

Note that we can find at max expectation value of other variables and not precise values, because to acquire precise value, we need eigen function of that dynamical ~~operator~~ variable's operator. The $\Psi(x)$ derived here is eigen function of only energy operator. Hence only precise value of Energy can be known.

Quantum Mechanics (5)

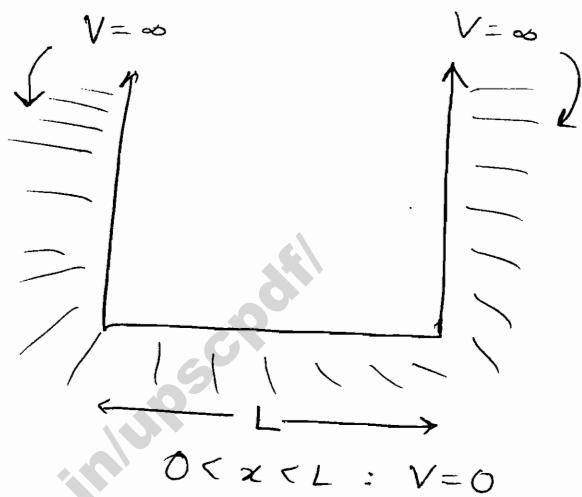
10/02/2012

$$\circ A\psi_n = (a_n) \psi_n$$

$$\text{Complete state} = |\psi\rangle = \sum c_i |\psi_i\rangle$$

Representation of $|\psi\rangle$
in Orthogonal vectors
of state space....
These are basis vectors

We have learnt, Particle in 1-d box i.e. inside infinite Potential Well



② Boundary Conditions due to ∞ potential

$$\psi(x=0) = 0$$

$$\psi(x=L) = 0$$

$$\text{For } 0 < x < L, \quad \frac{d^2\psi}{dx^2} + \frac{2mE}{\hbar^2} \psi = 0$$

Solution gives :

$$\psi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right)$$

$$E_n = n^2 \frac{\pi^2 \hbar^2}{2mL^2} = n^2 \frac{\hbar^2}{8mL^2}$$

$$n = 1, 2, 3, \dots$$

Complete picture emerges when we draw at least 3 states (minimum) of ψ and corresponding 3 levels of energy.

$$E_n = n^2 \left(\frac{\hbar^2}{8mL^2} \right) = n^2 \Delta \quad (\text{say})$$

Commensurate with de Broglie's wave : ✓

Commensurate with Heisenberg Principle:

$$E = \frac{p^2}{2m}$$

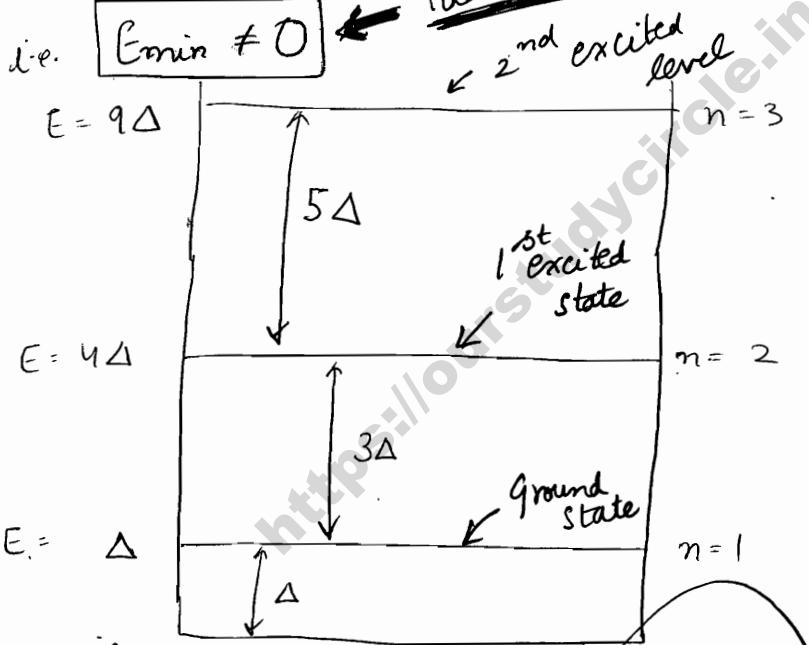
$$\Delta x \Delta p_x \geq \frac{\hbar}{2}$$

$$\Delta p_x \geq \frac{\hbar}{2L}$$

$$\Rightarrow p_x \geq \frac{\hbar}{2L}$$

$$E \geq \frac{\hbar^2}{4L^2} \cdot 2m = \frac{\hbar^2}{8mL^2}$$

$$E_{\min} = \frac{\hbar^2}{8mL^2}$$

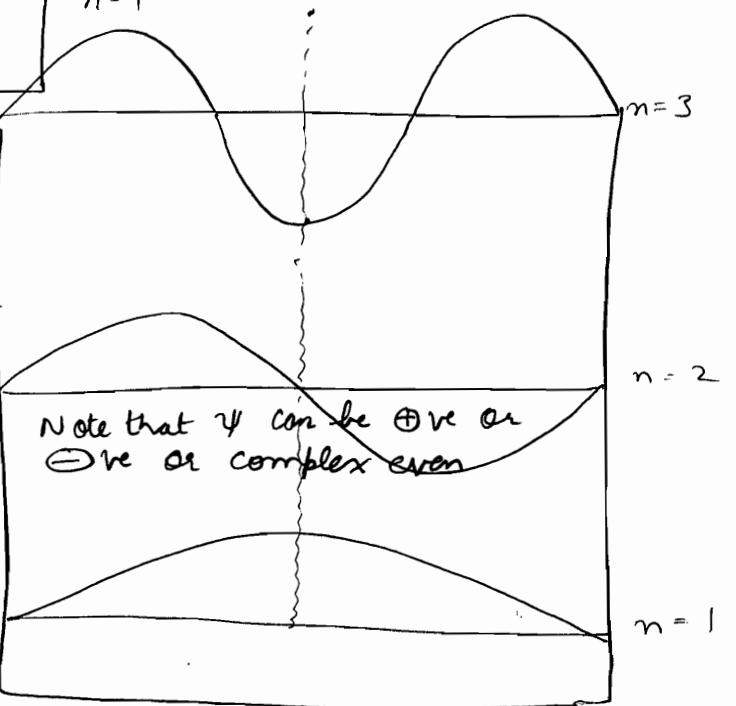


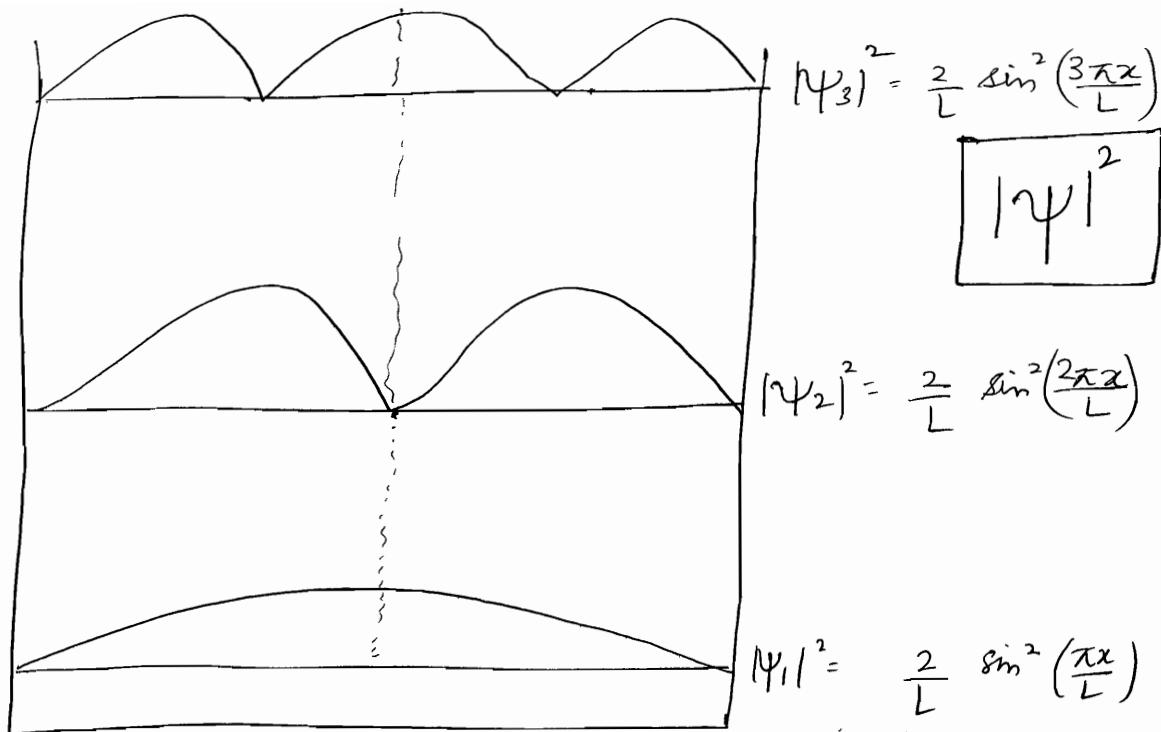
Remember in statistics, we used to talk about modes of energy as loops of standing waves. This is what we meant!!

$$\psi_2 = \sqrt{\frac{2}{L}} \sin\left(\frac{2\pi x}{L}\right)$$

$$\psi_1 = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi x}{L}\right)$$

$$\psi_3 = \sqrt{\frac{2}{L}} \sin\left(\frac{3\pi x}{L}\right)$$





n^{th} state $\Rightarrow n$ maxima of Probability [because $n =$ no. of loops]

If a particle is confined to $\psi = \sqrt{\frac{2}{L}} \sin\left(\frac{2\pi x}{L}\right)$
find out x for maximum probability.

$$P(x) = \psi \psi^* = \frac{2}{L} \sin^2\left(\frac{2\pi x}{L}\right)$$

For $P(x)$ maxima,

(What is meant by $\frac{d}{dx}$??)

$$\frac{d}{dx} \left[\frac{2}{L} \sin^2\left(\frac{2\pi x}{L}\right) \right] = 0 \quad \text{and } \left(\frac{d^2 P_x}{dx^2} \right) < 0$$

$$\frac{2}{L} \cdot 2 \sin\left(\frac{2\pi x}{L}\right) \cos\left(\frac{2\pi x}{L}\right) \cdot \left(\frac{2\pi}{L}\right) = 0$$

Expectation value
dice $\{1, 2, 3, 4, 5, 6\}$ \Rightarrow either $\sin\left(\frac{2\pi x}{L}\right) = 0 \Rightarrow x = \frac{n\pi L}{2\pi} = \left(\frac{n}{2}\right) L$
 $P_{\max} = \frac{1}{6} = \frac{1}{6}$

$$\cos\left(\frac{2\pi x}{L}\right) = 0 \Rightarrow x = \left(\frac{1}{4}(2n+1)\right) \left(\frac{\pi}{4} \cdot L\right)$$

$$\frac{d^2 x}{dx^2} = \cos\left(\frac{4\pi x}{L}\right) = \text{negative for } x = (2n+1) \frac{L}{4}$$

Note that we have to find out both the derivatives. Otherwise, answer will not be complete.

Show that the result is commensurate with Heisenberg uncertainty principle.

$$\psi_x = \sqrt{\frac{2}{L}} \sin\left(\frac{2\pi x}{L}\right)$$

$$\text{To prove } \Delta x \Delta p_x \geq \frac{\hbar}{2}$$

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

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

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

$$= \frac{1}{L} \int_0^L x \left(1 - \cos \frac{4\pi x}{L}\right) dx$$

$$= \frac{1}{L} \left[\frac{L^2}{2} - \left[\int_0^L x \cos \left(\frac{4\pi x}{L} \right) \right] \right] = \underline{\underline{\left(\frac{L}{2} \right)}}$$

Similarly $\langle x^2 \rangle = \frac{1}{L} \int_0^L x^2 \left(1 - \cos \frac{4\pi x}{L}\right) dx = \underline{\underline{\left(\frac{L^2}{3} \right)}}$

$$\langle p_x \rangle = \langle \psi | P_x | \psi \rangle$$

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

$$= 0$$

Note
this
term
also

$$\rightarrow -\frac{L^2}{8\pi^2}$$

$$\langle \hat{p}_x \rangle = 0$$

Almost Always ... (when ψ is real)

$\langle \hat{p}_x^2 \rangle \neq 0$ otherwise $T=0$ which is never the case.

$$\langle \hat{p}_x^2 \rangle = \langle \psi | \hat{p}_x^2 | \psi \rangle$$

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

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

$$= \frac{2\hbar^2}{L} \cdot \frac{n^2\pi^2}{L^2} \cdot \int_0^L \frac{1 - \cos\left(\frac{2n\pi x}{L}\right)}{2} dx$$

$$= \frac{2\hbar^2 \cdot n^2\pi^2}{L^3} \cdot \frac{L}{2}$$

$$= \cancel{\left(\frac{\hbar^2 n^2 \pi^2}{L^3}\right)} \quad \underline{\left(\frac{\hbar^2 n^2 \pi^2}{L^2}\right)}$$

Easy way

$$\langle H \rangle = \frac{n^2 \hbar^2}{8mL^2}$$

as it is eigenstate
of Hamiltonian

But for free particle

$$\langle H \rangle = \langle \frac{\hat{p}^2}{2m} \rangle = \frac{1}{2m} \langle \hat{p}^2 \rangle$$

$$\Rightarrow \langle \hat{p}^2 \rangle = 2m \cdot \frac{n^2 \hbar^2}{8mL^2}$$

$$= \frac{(n^2 \hbar^2)}{(4L^2)}$$

$$\Delta p = \sqrt{\langle \hat{p}^2 \rangle - \langle \hat{p} \rangle^2} \\ = \underline{\underline{\frac{(m\hbar)^2}{(2L)}}}$$

$$\Rightarrow \Delta p_x = \cancel{\left(\frac{n\pi\hbar}{L}\right)} \quad \underline{\left(\frac{n\pi\hbar}{L}\right)}$$

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

$$= \sqrt{\frac{L^2}{3} - \frac{L^2}{4}} = \sqrt{\frac{L^2}{12}}$$

$$\Delta p_x \Delta x = \frac{n\pi\hbar}{L} \cdot \frac{L}{\sqrt{12}} \Rightarrow \frac{\pi\hbar}{\sqrt{12}} = \underline{\underline{\left(\frac{\hbar}{\sqrt{12}}\right)}} > \underline{\underline{\left(\frac{\hbar}{2}\right)}}$$

$$\langle T \rangle = \frac{\langle p_x^2 \rangle}{2m} = \frac{n^2 \frac{h^2}{4L^2}}{2m} = n^2 \left(\frac{h^2}{8mL^2} \right)$$

* Since we have calculated precise value of T , $\langle T \rangle$ = same as the value calculated.

~~Q1~~ If $\psi_x = \frac{1}{\sqrt{14}} \phi_1(x) + \frac{2}{\sqrt{14}} \phi_2(x) + \frac{3}{\sqrt{14}} \phi_3(x)$

and Particle is trapped in 1-d box.

Find $\langle E \rangle$.

refer Q1 - P 152
of verma

Wave Function represents only Probability

If there is summation in ψ
 \Rightarrow either it can be in state 1 or state 2 or state 3

If $|\psi_{\alpha}\rangle = c_1 \phi_1 + c_2 \phi_2 + c_3 \phi_3$

If normalized $\Rightarrow \langle \psi | \psi \rangle = 1 \Rightarrow \langle c_1 \phi_1 + c_2 \phi_2 + c_3 \phi_3 | c_1 \phi_1 + c_2 \phi_2 + c_3 \phi_3 \rangle = 1$

$\Rightarrow \underbrace{\langle c_1 \phi_1 | \psi \rangle}_{c_1^* c_1} + \underbrace{\langle c_2 \phi_2 | \psi \rangle}_{c_2^* c_2} + \underbrace{\langle c_3 \phi_3 | \psi \rangle}_{c_3^* c_3} = 1$

$c_1^* c_1 \underbrace{\langle \phi_1 | \phi_1 \rangle}_{= 1} + c_2^* c_2 \underbrace{\langle \phi_2 | \phi_2 \rangle}_{= 0} + c_3^* c_3 \underbrace{\langle \phi_3 | \phi_3 \rangle}_{= 0} = 1$
 $c_1^* c_1 = |c_1|^2$
 $(\text{kronecker } \delta \text{ function})$

$\Rightarrow |c_1|^2 + |c_2|^2 + |c_3|^2 = 1$

Now

$$|\psi_x\rangle = c_1 \phi_1 + c_2 \phi_2 + c_3 \phi_3$$

$$\langle \phi_i | \psi \rangle = \langle \phi_i | c_1 \phi_1 \rangle = c_1$$

Probability of Measurement in any state $\phi_i = |c_i|^2$

$$\text{Prob.} = |\langle \phi_i | \psi \rangle|^2$$

$$\begin{aligned}\langle E \rangle &= \langle \psi | H | \psi \rangle / \langle \psi | \psi \rangle \\ &= \frac{1}{14} \langle \phi_1 | H | \phi_1 \rangle + \frac{4}{14} \langle \phi_2 | H | \phi_2 \rangle \\ &\quad + \frac{9}{14} \langle \phi_3 | H | \phi_3 \rangle\end{aligned}$$

★ Note that for deep well wave functions ϕ_1, ϕ_2, \dots

$$\langle \phi_1 | H | \phi_2 \rangle = 0$$

but

$$\langle \phi_1 | x | \phi_2 \rangle \neq 0$$

[We know $\langle \psi_n | H | \psi_n \rangle$]

$$= n^2 \frac{\hbar^2}{8mL^2}$$

Hence this method won't work if $\langle x \rangle$ is asked then we need to find $\langle \phi_1 | x | \phi_2 \rangle$ also....

$$\begin{aligned}\langle E \rangle &= \frac{1}{14} \cdot \left(\frac{\hbar^2}{8mL^2} \right) + \frac{4}{14} \cdot 4 \left(\frac{\hbar^2}{8mL^2} \right) + \frac{9}{14} \cdot 9 \left(\frac{\hbar^2}{8mL^2} \right) \\ &= \frac{1+16+81}{14} \cdot \frac{\hbar^2}{8mL^2} = \frac{98}{14 \cdot 8} \cdot \frac{\hbar^2}{mL^2}\end{aligned}$$

$$\langle E \rangle = \left(\frac{7 \hbar^2}{8mL^2} \right) \checkmark$$

Infinite Energy Well Problem with changed coordinates.

$$|x| < \frac{a}{2} \quad V = 0$$

$$|x| > \frac{a}{2} \quad V = \infty$$

Writing the eqn,

$$\frac{d^2 \psi_1}{dx^2} + \frac{2mE}{\hbar^2} \psi_1 = 0$$

$$\Rightarrow \psi_1 = A \sin kx + B \cos kx$$

$$\Pi [f(x)] = f(\bar{x})$$

if $\Pi[H\psi(x)] = H[\Pi\psi(x)]$

→ common eigenfunctions

→ energy eigenfunctions $= \frac{\alpha}{2}$
= odd or even

$$x = \left(\frac{\alpha}{2} \right)$$

Hamiltonian

with

commutes
Function
Parity if V is even

Boundary Conditions

$$\psi(x = -\frac{a}{2}) = 0 = \psi(x = +\frac{a}{2})$$

$$\Rightarrow -A \sin \frac{ka}{2} + B \cos \frac{ka}{2} = 0$$

$$A \sin \frac{ka}{2} + B \cos \left(\frac{ka}{2}\right) = 0$$

Adding $\Rightarrow B \cos \left(\frac{ka}{2}\right) = 0 \quad \dots \textcircled{1}$

Subtracting $\Rightarrow A \sin \left(\frac{ka}{2}\right) = 0 \quad \dots \textcircled{2}$

Refer Ch-13
to understand
rationale behind
closed form
of solutions

From ①

either $B = 0$

$$\Rightarrow \psi_1 = A \sin(kx)$$

or

$$\cos \left(\frac{ka}{2}\right) = 0$$

From ②

either $A = 0$

or

$$\sin \left(\frac{ka}{2}\right) = 0$$

$$\Rightarrow \psi_2 = B \cos kx$$

Closed Form Solutions

are solutions.

\Rightarrow Both $A \sin kx$ and $B \cos kx$

In such a case, a single solution cannot satisfy all the possible cases. Hence we require both solutions, each catering to different cases.

~~$$\psi = A \sin kx$$~~

$$\psi(x = \pm \frac{a}{2}) = 0$$

$$\Rightarrow k \frac{a}{2} = n\pi \Rightarrow k = \left(\frac{2n\pi}{a}\right)$$

$$n = 1, 2, 3, \dots$$

$$E_n = \frac{\hbar^2 k^2}{2m} = \frac{\hbar^2}{2m} \left(\frac{2n\pi}{a} \right)^2 = (2n)^2 \left(\frac{\hbar^2 \pi^2}{2ma^2} \right) = (2n)^2 \left(\frac{\hbar^2}{8ma^2} \right)$$

$\psi = B \cos kx$

$$\cos \frac{ka}{2} = 0$$

$$\frac{ka}{2} = (2n-1) \frac{\pi}{2} \Rightarrow k = (2n-1) \frac{\pi}{a}$$

$$E_n = \frac{\hbar^2 k^2}{2m} = (2n-1)^2 \left(\frac{\hbar^2 \pi^2}{2ma^2} \right) = (2n-1)^2 \left(\frac{\hbar^2}{8ma^2} \right)$$

Upon Normalization $A=B=\sqrt{\frac{2}{L}}$

Also note that we always like to start our states from +1 hence we use $(2n-1)$

This way we should write down final equation!!

$$\Rightarrow \boxed{\psi_{1n} = \sqrt{\frac{2}{a}} \cos \left[\frac{(2n-1)\pi}{a} x \right] \Rightarrow E_{1n} = (2n-1)^2 \left(\frac{\hbar^2 \pi^2}{2ma^2} \right)}$$

$$\boxed{\psi_{2n} = \sqrt{\frac{2}{a}} \sin \left[\frac{2n\pi}{a} x \right] \Rightarrow E_{2n} = (2n)^2 \left(\frac{\hbar^2 \pi^2}{2ma^2} \right)}$$

Final solution are represented in terms of Quantum Numbers

We can combine the 2 solutions as

$$\psi_n = \sqrt{\frac{2}{a}} \left[\sin \left(\frac{2n\pi x}{a} \right) + \cos \left(\frac{(2n-1)\pi x}{a} \right) \right] \text{ do not write like this !!}$$

$$E_n = n^2 \left(\frac{\hbar^2 \pi^2}{2ma^2} \right)$$

[Odd squares or even squares
⇒ all integral squares]

$$\underline{\text{Q19}} \quad \Psi(q, t) = \psi(q, 0) e^{-i\omega t} = A e^{-i\omega t}$$

Expansion Coefficient

$$\left[\begin{array}{l} F(k) = \frac{1}{\sqrt{2\pi}} \int f(x) e^{-ikx} dx \\ \text{Fourier} \\ f(x) = \frac{1}{\sqrt{2\pi}} \int F(k) e^{ikx} dk \end{array} \right] \text{Not required}$$

Normalization

$$\int_a^a \psi^* \psi dq = |A|^2 a = 1$$

$$\Rightarrow |A| = \frac{1}{\sqrt{a}}$$

$$\Rightarrow \psi(q, t) = \frac{1}{\sqrt{a}} e^{-i\omega t}$$

$$\begin{aligned} F(k) &= \frac{1}{\sqrt{2\pi}} \int_0^a \frac{1}{\sqrt{a}} e^{-i(\omega t + kx)} dx \\ &= \frac{1}{\sqrt{2\pi a}} \left[\frac{e^{-i(\omega t + kx)}}{-ik} \right]_0^a \end{aligned}$$

Note that we do not require time here, put $t=0$

$$\begin{aligned} F(k) &= \frac{1}{\sqrt{2\pi a}} \left[\frac{e^{-ikx}}{-ik} \right]_0^a \\ &= \frac{1}{\sqrt{2\pi a}} \frac{e^{-ika} - 1}{-ik} \end{aligned}$$

Q2a) $H\psi = E\psi$

$i\hbar \frac{\partial \psi}{\partial t} = E\psi$ — time dependent
form of Schrödinger
solution

$$\Rightarrow \ln \psi = \frac{Et}{i\hbar} + \ln A$$

$$\psi = A e^{-\left(\frac{iEt}{\hbar}\right)}$$

Q30)

$$\boxed{\begin{array}{l} 3^{\text{rd}} \text{ excited: } n=4 \\ \text{ground: } n=1 \end{array}}$$

This was taught by
P. Bahadur

$$\Delta E = E_4 - E_1 = (16-1) \frac{\hbar^2}{8mL^2} = \frac{15 \hbar^2}{8mL^2}$$

$$\Rightarrow 60 \text{ eV} = \frac{15 \hbar^2}{8mL^2}$$

$$\Rightarrow L^2 = \frac{15 \times (6.62)^2 \times 10^{-68}}{8 \times 9.1 \times 10^{-31} \times 60 \times 1.6 \times 10^{-19}} \\ = 0.094 \times 10^{-18}$$

$$L = 0.306 \times 10^{-9}$$

$$= \underline{0.3 \text{ nm}}$$

<https://ourstudycircle.in/upscpdf/>

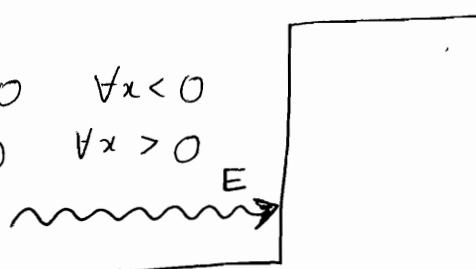
Quantum Physics (6)

11/02/12

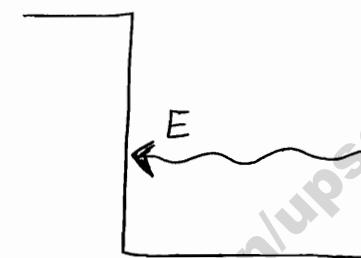
Problem of Step Potential

$$V \leq 0 \quad \forall x < 0$$

$$V > 0 \quad \forall x > 0$$



(Ascending
step
potential)



(descending step
potential)

① We need to work out

$$T = \frac{J_T}{J_I} = \frac{\text{Transmitted Flux}}{\text{Incident Flux}}$$

Reflection = fraction of particles reflected

$$R = \frac{J_R}{J_I} = \frac{\text{Reflected Flux}}{\text{Incident Flux}}$$

Transmittance
= fraction of particle
transmitted

$$\text{We know } J = \frac{\hbar}{2mi} \left[\psi^* \frac{\partial \psi}{\partial x} - \psi \frac{\partial \psi^*}{\partial x} \right]$$

Hence to calculate coefficients we need to find out functions

ψ_I, ψ_R, ψ_T

We have Schrodinger Wave Equation at our disposal.

$$\text{For } x < 0 \quad H \psi_I = E \psi_I$$

$$\Rightarrow \frac{d^2 \psi_I}{dx^2} + \frac{2m(E-V)}{\hbar^2} \psi_I = 0$$

$$\Rightarrow \frac{d^2 \psi_I}{dx^2} + \frac{2mE}{\hbar^2} \psi_I = 0$$

$$\Rightarrow \Psi_1 = A e^{i k_1 x} + B e^{-i k_1 x}$$

$$k_1^2 = \frac{2mE}{\hbar^2}$$

For $x > 0$

$$\frac{d^2 \Psi_2}{dx^2} + \frac{2m}{\hbar^2} (E - V_0) \Psi_2 = 0$$

here we have two cases, either $E > V_0$
or
 $E < V_0$

CASE 1

$$E > V_0$$

Classically Feasible Case....

Quantum Mechanically non important case....

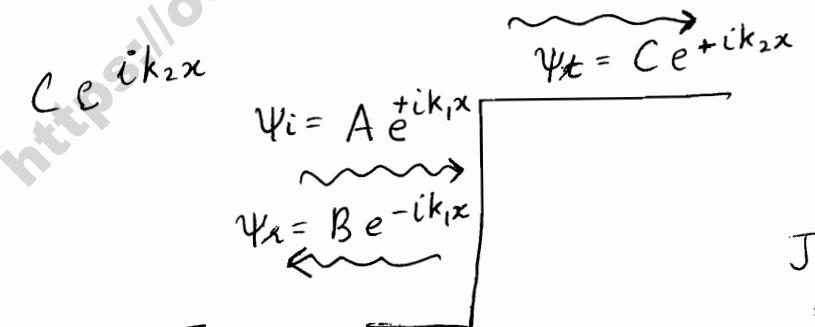
$$\frac{d^2 \Psi_2}{dx^2} + \frac{2m}{\hbar^2} (E - V_0) \Psi_2 = 0$$

$$\Rightarrow \frac{d^2 \Psi_2}{dx^2} + k_2^2 \Psi_2 = 0 \quad \text{where } k_2^2 = \frac{2m}{\hbar^2} (E - V_0)$$

$$\Psi_2 = C e^{i k_2 x} + D e^{-i k_2 x}$$

Note that when particle is transmitted, no returning back
i.e. $D = 0$

$$\Rightarrow \Psi_2 = C e^{i k_2 x}$$



Step 1 Calculating J

$$\begin{aligned} J &= p v \\ &= |\Psi|^2 \cdot \frac{\hbar}{m} \\ &= \frac{|\Psi|^2 \hbar k}{m} \quad (\text{for exp}) \end{aligned}$$

$$J_x = \frac{\hbar}{2mi} \left[A^* e^{-ik_1 x} A e^{ik_1 x} (ik_1) + A e^{ik_1 x} A^* e^{-ik_1 x} (ik_1) \right]$$

$$= \frac{\hbar}{2mi} 2 A A^* k_i = \frac{\hbar k_1 A A^*}{m} = \frac{\hbar k_1 |A|^2}{m}$$

$$J_i = \frac{k_1 \hbar |A|^2}{m}$$

Similarly,

$$J_R = \frac{k_1 \hbar |B|^2}{m}$$

$$J_T = \frac{k_2 \hbar |C|^2}{m}$$

Reflectance or

R: fraction of particles reflected

T: fraction of particles transmitted

or

Transmittance

$$R = \frac{BB^*}{AA^*}$$

$$T = \frac{k_2 CC^*}{k_1 AA^*}$$

Step II Applying Boundary Conditions

~~Boundary conditions~~

$$\psi_1 = \psi_2$$

(Single valued Function)

$$\Rightarrow A + B = C \quad \dots \quad (1)$$

$$\left. \frac{d\psi_1}{dx} \right|_{x=0} = \left. \frac{d\psi_2}{dx} \right|_{x=0}$$

(Continuous at $x=0$)

$$\Rightarrow ik_1(A - B) = ik_2 C \quad \dots \quad (2)$$

From (1) and (2),

$$A = \left(1 + \frac{k_2}{k_1}\right) \frac{C}{2}$$

$$B = \left(1 - \frac{k_2}{k_1}\right) \frac{C}{2}$$

$$\Rightarrow \left(\frac{B}{A}\right) = \frac{1 - \frac{k_2}{k_1}}{1 + \frac{k_2}{k_1}} \quad ; \quad \left(\frac{C}{A}\right) = \frac{2k_1}{k_1 + k_2}$$

$$R = \left(\frac{k_1 - k_2}{k_1 + k_2} \right)^2$$

$$T = \frac{4 k_1 k_2}{(k_1 + k_2)^2}$$

$$\underline{R + T = 1}$$

Fraction of flux reflected

Fraction of flux transmitted

~~Q1)~~

$$\frac{\hbar k_1}{m} |A|^2 = 1$$

$$|A| = \sqrt{\frac{m}{\hbar k_1}}$$

$$R = \left(\frac{1 - \sqrt{\frac{E - V_0}{E}}}{1 + \sqrt{\frac{E - V_0}{E}}} \right)^2 \quad \star$$

$$E - V_0 = 1$$

$$E = 1.5$$

$$= \left(\frac{1 - \sqrt{\frac{2}{3}}}{1 + \sqrt{\frac{2}{3}}} \right)^2 \approx \frac{1}{81}$$

$$T = 1 - R$$

$$R = \frac{J_x}{J_i}, \quad T = \frac{J_t}{J_i}$$

$$\Rightarrow J_x = R \cdot J_i, \quad J_t = T \cdot J_i$$

CASE 2

$E < V_0$

Classically Forbidden Case
Quantum Mechanically Important Case

Region 1

$$\psi = \underline{A e^{ik_1 x}} + \underline{B e^{-ik_1 x}}$$

$$k_1 = \sqrt{\frac{2mE}{\hbar^2}}$$

Region 2

Step I

$$\frac{d^2\psi_2}{dx^2} - \frac{2m}{\hbar^2} (V_0 - E) \psi_2 = 0$$

$$\Rightarrow \frac{d^2\psi_2}{dx^2} - k_2^2 \psi_2 = 0$$

$$k_2 = \sqrt{\frac{2m(V_0 - E)}{\hbar^2}}$$

In this region, it is called CLASSICALLY FORBIDDEN REGION.

$$\psi_2 = C e^{-k_2 x} + D e^{k_2 x}$$

Note that these are not returning or going waves...
these are decreasing amplitude functions.....

Finiteness on ψ_2 : $D = 0$

(as $x \rightarrow \infty$
 $\psi_2 \rightarrow 0$)

$$\Rightarrow \psi_2 = \underline{C e^{-k_2 x}}$$

$$J_i = \frac{\hbar k_1 |A|^2}{m}$$

$$J_r = \frac{\hbar k_1 |B|^2}{m}$$

$$J_t = 0$$

Step II : Boundary Conditions

$$\text{Single valued} : A + B = C$$

Continuity

$$\left. \frac{d\psi_1}{dx} \right|_{x=0} = \left. \frac{d\psi_2}{dx} \right|_{x=0} \Rightarrow$$

$$A - B = -\frac{k_2}{k_1} C = i \frac{k_2}{k_1} C$$

$$\text{Adding} \quad A = \left(1 + i \frac{k_2}{k_1}\right) \frac{C}{2}$$

$$\text{Subtracting} \quad B = \left(1 - i \frac{k_2}{k_1}\right) \frac{C}{2}$$

$$R = \frac{|B|^2}{|A|^2} = \left| \frac{1 - \frac{ik_2}{k_1}}{1 + ik_2} \right|^2 \Rightarrow R = \frac{BB^*}{AA^*} = 1$$

$$T = \frac{J_T}{J_C} = 0$$

~~Both~~ $k_1 < k_2$

* But $|C|^2 \neq 0$

$$J_t = \frac{\hbar}{2mi} \left[\psi_t^* \frac{\partial \psi_t}{\partial x} - \psi_t \frac{\partial \psi_t^*}{\partial x} \right]$$

$$= \frac{\hbar}{2mi} \left[C^* C e^{-2k_2 x} - C C^* e^{-2k_2 x} \right]$$

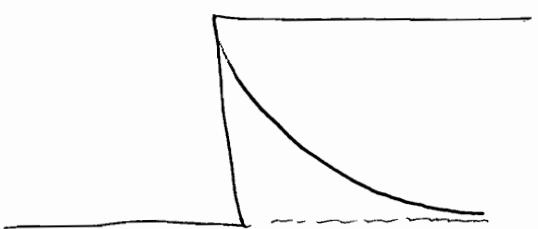
$$= 0$$

$\Rightarrow T$ should be 0

→ This is what we expected classically

but $C \neq 0$

i.e. there is some probability of particle being in Region 2.



$$P = |C|^2 e^{-2k_2 x}$$

$$P_{max} = |C|^2 \text{ at } x=0$$

$$\text{Prob} = \frac{P_{max} e^{-2k_2 x}}{P_{max}}$$

i.e. even when no particle is crossing, there is some probability of particle being present there.

Penetration Depth : ★ distance from barrier where wave function falls to $\frac{1}{e}$ times its max.

$$\psi_d = \frac{1}{e} \psi_{\max} \quad \boxed{\text{value}}$$

$$\Rightarrow C e^{-k_2 d} = \frac{1}{e} \cdot C$$

$$\Rightarrow \boxed{d = \left(\frac{1}{k_2} \right) : \text{Penetration depth}}$$

i.e. upto this distance only, function is significant across the potential. Afterwards, it is negligible.

This is a consequence of Heisenberg's Uncertainty Principle. Whatever I call, $x=0$, there is some error in measurement.

$$\Delta x = d \quad (\text{Penetration Depth})$$

Find Δx
by taking $\psi = Ce^{-kx}$

$$\hbar x = \hbar k_2$$

$$\Delta \hbar x = \hbar k_2$$

$$\Delta x = \frac{\hbar}{\hbar k_2} = \frac{1}{k_2} = \text{Penetration depth}$$

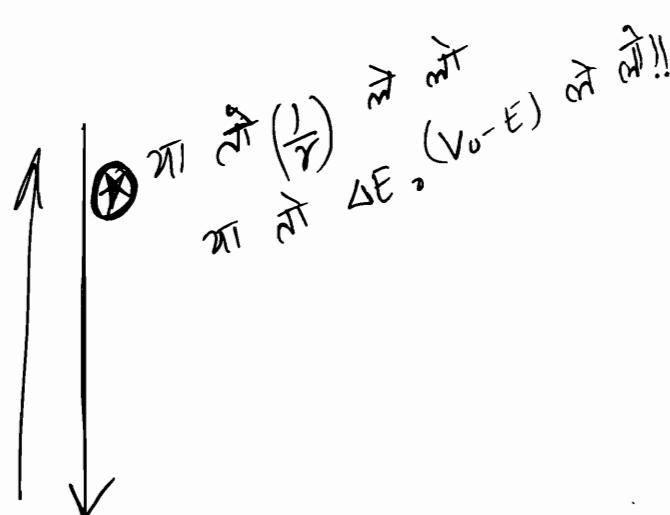
if $E = E + \Delta E$

$$\Rightarrow \Delta E = V_0 - E$$

$$\frac{\Delta \hbar x^2}{2m} = (V_0 - E)$$

$$\Delta \hbar x = \sqrt{2m(V_0 - E)}$$

$$\Delta x = \frac{\hbar}{\sqrt{2m(V_0 - E)}} = \underline{\underline{\left(\frac{1}{r} \right)}}$$



Particle in a 3-d box or Cubical Box

① Length of side = L

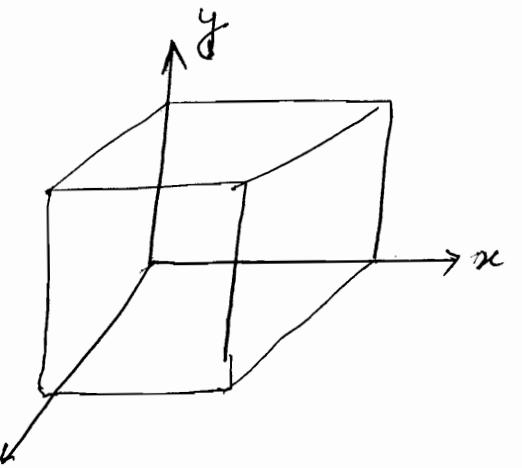
② Particle of mass m,
trapped in 3-d Box.

Free to move between

$$x: 0 \text{ to } L$$

$$y: 0 \text{ to } L$$

$$z: 0 \text{ to } L$$



Note that it cannot remain on walls.

$$\psi(x=0) = 0 = \psi(x=L_x)$$

$$\psi(y=0) = 0 = \psi(y=L_y)$$

$$\psi(z=0) = 0 = \psi(z=L_z)$$

$V=0$ inside the box.

$$\Rightarrow E = T$$

Using Schrodinger Wave Equation,

$$H\psi = E\psi$$

$$\Rightarrow -\frac{\hbar^2}{2m} \nabla^2 \psi = E\psi$$

$$\Rightarrow \boxed{\nabla^2 \psi + \frac{2mE}{\hbar^2} \psi = 0}$$

$$\frac{2mE}{\hbar^2} = \frac{k^2}{\hbar^2} = \frac{\hbar^2 k^2}{\hbar^2} = k^2$$

★ Again we see that k is our usual wave no. corresponding to de broglie wave!!

$$\Rightarrow \nabla^2 \psi + k^2 \psi = 0$$

$$\Rightarrow (\nabla^2 + k^2) \psi = 0$$

In 3 dimension,

*(Writing k as a composition
of 3-dimensional k -space)*

$$\left[\frac{\partial^2 \psi}{\partial x^2} + \frac{\partial^2 \psi}{\partial y^2} + \frac{\partial^2 \psi}{\partial z^2} \right] + [k_x^2 + k_y^2 + k_z^2] \psi = 0$$

Such Partial derivative equation is always worked out by separation of variables

$$\psi(x, y, z) = X(x) Y(y) Z(z)$$

$$\Rightarrow \frac{\partial \psi}{\partial x} = YZ \frac{\partial X}{\partial x} = YZ \frac{dX}{dx}$$

\Rightarrow in equation,

$$YZ \frac{d^2 X}{dx^2} + XZ \frac{d^2 Y}{dy^2} + XY \frac{d^2 Z}{dz^2} + (k_x^2 + k_y^2 + k_z^2) XYZ = 0$$

divide by XYZ

$$\Rightarrow \left[\frac{1}{X} \frac{d^2 X}{dx^2} + k_x^2 \right] + \left[\frac{1}{Y} \frac{d^2 Y}{dy^2} + k_y^2 \right] + \left[\frac{1}{Z} \frac{d^2 Z}{dz^2} + k_z^2 \right] = 0$$

all brackets should be individually 0.

Considering solution along X -axis,

$$\frac{1}{X} \frac{d^2 X}{dx^2} + k_x^2 = 0$$

$$\frac{d^2X}{dx^2} + k_x^2 X = 0$$

This is similar to 1-d.

$$X(x) = \sqrt{\frac{2}{L_x}} \sin(k_x x)$$

do not write $\sqrt{\frac{2}{L_x}}$ as we cannot yet normalize $X(x)$
 \therefore its not a wave function

at $x=L$,

$$X(L)=0 = \sqrt{\frac{2}{L_x}} \sin(k_x L) \Rightarrow n_x \pi = k_x L$$

$$\Rightarrow k_x = \frac{n_x \pi}{L_x}$$

$$k_y = \frac{n_y \pi}{L_y}$$

$$k_z = \frac{n_z \pi}{L_z}$$

$$\Rightarrow X(x) = \sqrt{\frac{2}{L_x}} \sin\left(\frac{n_x \pi}{L_x} x\right)$$

$n_x = 1, 2, 3, \dots$

$$Y(y) = \sqrt{\frac{2}{L_y}} \sin\left(\frac{n_y \pi}{L_y} y\right)$$

$$Z(z) = \sqrt{\frac{2}{L_z}} \sin\left(\frac{n_z \pi}{L_z} z\right)$$

Similarly,

$$\Psi(x, y, z) = \sqrt{\frac{8}{L_x L_y L_z}} \sin\left(\frac{n_x \pi x}{L_x}\right) \sin\left(\frac{n_y \pi y}{L_y}\right) \sin\left(\frac{n_z \pi z}{L_z}\right)$$

Also

$$k_x^2 + k_y^2 + k_z^2 = k^2 = \frac{2m E^*}{\hbar^2}$$

$$\left[\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2} \right] = \frac{2m E^*}{\pi^2 \hbar^2}$$

① Here @ this step, we can normally and easily obtain $\sqrt{\frac{8}{L_x L_y L_z}}$ as 3. Integrations will be separated out easily.

$$\Rightarrow E_{(n_x, n_y, n_z)} = \frac{\hbar^2 \pi^2}{2m} \left[\frac{n_x^2}{L_x^2} + \frac{n_y^2}{L_y^2} + \frac{n_z^2}{L_z^2} \right]$$

$$E_r \propto |k_r|^2 = (k_x^2 + k_y^2 + k_z^2)$$

For cubical box, $\Delta = \frac{\hbar^2}{8mL^2}$

$E_{(n_x, n_y, n_z)} = \frac{\hbar^2 \pi^2}{2m L^2} [n_x^2 + n_y^2 + n_z^2]$

eigen values $\Psi(x, y, z) = \sqrt{\frac{8}{L^3}} \sin\left(\frac{n_x \pi x}{L}\right) \sin\left(\frac{n_y \pi y}{L}\right) \sin\left(\frac{n_z \pi z}{L}\right)$

Any off the 3 quantum numbers, $n_x, n_y, n_z \neq 0$

If any 1 is 0 \Rightarrow 2-d motion

If any 2 are 0 \Rightarrow 1-d motion

Note that (1, 1, 1) is the minima.

n corresponds to number of loops !!!

(as in 1-d case)



g_i : space degeneracy

$$H\Psi = E\Psi$$

$$H\Psi(1,1,1) = 3\Delta\Psi(1,1,1)$$

$$E = 14\Delta$$

$$\Psi(1, 2, 3) \quad g_6 = 6$$

$$\left. \begin{array}{l} \text{3 degenerate states i.e.} \\ \text{same eigen value} \end{array} \right\} H\Psi(2, 1, 1) = 6\Delta\Psi(2, 1, 1)$$

$$E = 12\Delta$$

$$\Psi(2, 2, 2) \quad g_5 = 1$$

$$H\Psi(2, 2, 1) = 6\Delta\Psi(2, 2, 1)$$

$$E = 11\Delta$$

$$\Psi(3, 1, 1) \text{ or } \Psi(1, 3, 1) \text{ or } \Psi(1, 1, 3) \quad g_4 = 3$$

$$E = 9\Delta$$

$$\Psi(2, 2, 1) \text{ or } \Psi(2, 1, 2) \text{ or } \Psi(1, 3, 2) \quad g_3 = 3$$

$$E = 6\Delta$$

$$\Psi(2, 1, 1) \text{ or } \Psi(1, 2, 1) \text{ or } \Psi(1, 1, 2) \quad g_2 = 3$$

$$E = 3\Delta$$

$$\Psi_{(1,1)} = \sqrt{\frac{8}{L^3}} \sin\left(\frac{\pi x}{L}\right) \sin\left(\frac{\pi y}{L}\right) \sin\left(\frac{\pi z}{L}\right) \quad g_1 = 1$$

$g_1 = 1$: non degenerate state

$g_2 = 3$: degenerate state

If there are n independent functions corresponding to 1 eigen value $\Rightarrow n$ -fold degeneracy.

In Maxwell-Boltzmann or Bose Einstein, we can put all particles in a single state.

But in Fermi Dirac (electrons), only 1 e⁻ in 1 state.

Note that these states are of kinetic energy (p_x^2, p_y^2, p_z^2) only. We have not taken spin into account.

degeneracy factor is multiplication of space degeneracy & spin degeneracy

$$g = g_{\text{space}} * g_{\text{spin}} = g_i (2s+1)$$

example: I have to fill 10 e⁻ without taking spin into account.

Energy (no. of e⁻)



$$3\Delta(1) + 6\Delta(3) + 9\Delta(3) + 11\Delta(3)$$

Taking spin into consideration, $(1, 1, 1, \frac{1}{2})$
 $(1, 1, 1, -\frac{1}{2})$

$$3\Delta(2) + 6\Delta(6) + 9\Delta(2)$$

Tut 3
Q 15

Density of States

We know,

$$E = \frac{\pi^2 \hbar^2}{2mL^2} (n_x^2 + n_y^2 + n_z^2)$$

$$\text{Let } \left(\frac{2mL^2}{\pi^2 \hbar^2} \right) E = R^2 = n_x^2 + n_y^2 + n_z^2$$

$$R = \frac{1}{\pi \hbar} \sqrt{2mE}$$

$$\underline{n_x^2 + n_y^2 + n_z^2 = R^2}$$

↑
Sphere of radius R

density of states

$$g = \frac{dN}{dE}$$

$$N(E) = \int_0^E g(E) dE$$

$$n_x, n_y, n_z \rightarrow E$$

$$n_x + dn_x, n_y + dn_y, n_z + dn_z \rightarrow E + dE$$

$dN = N$ - of energy states between E and $E+dE$ are energy states lying between radius : R and $R+dE$

= Volume of sphere b/w R and $(R+dE)$

[Note that Quantum Numbers are POSITIVE] \Rightarrow only 1 octant

④ do not get confused

Previous 'g' was degeneracy

This 'g' is density of state

refer P-311

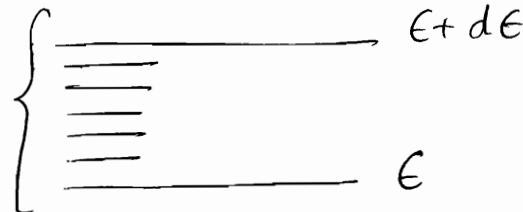
④ Change in Energy corresponds to change in k which corresponds to change in radius of sphere $k^2 = k_x^2 + k_y^2 + k_z^2$

We need to find dN where k changes from k to $k + dk$ where Energy is related to states

N = No. of states as

$$E = \frac{n^2 \hbar^2}{2mL^2} (n_x^2 + n_y^2 + n_z^2)$$

1 quantum state per $\left(\frac{\pi}{L}\right)^3$ volume.



$$\Rightarrow dN = \frac{dV}{dV} = \frac{4}{3} \frac{\pi k^2 dk}{\left(\frac{\pi}{L}\right)^3}$$

$$= \frac{1}{8} \text{ (Volume difference)}$$

$$\begin{aligned} &= \frac{1}{8} \left[\frac{4\pi}{3} (R + dR)^3 - \frac{4\pi}{3} R^3 \right] \\ &= \frac{1}{8} \cdot 4\pi R^2 dR \\ &= \frac{4\pi R^2 dR}{3} \end{aligned}$$

Now we know,

$$R = \frac{L}{\pi \hbar} \sqrt{2mE}$$

$$\Rightarrow dR = \cancel{\frac{L}{\pi \hbar} \sqrt{2mE}} = \frac{L}{\pi \hbar} \sqrt{\frac{m}{2E}} dE$$

$$\Rightarrow dN = \frac{1}{8} \cdot 4\pi \cdot \frac{L^2}{\pi^2 \hbar^2} \cdot 2mE \cdot \frac{1}{2} \cdot \frac{L}{\pi} \cdot \frac{\sqrt{2m}}{\sqrt{E}\hbar} dE$$

$$= \frac{4\pi}{16} \cdot \frac{L^3}{\pi^3 \hbar^3} (2m)^{3/2} E^{1/2} dE$$

○ तरे मया !! $g(E)$ को

density of state
बोलते हैं !!

$$dN(E) = \frac{2\pi V}{\hbar^3} (2m)^{3/2} E^{1/2} dE$$

$$dN = g(E) dE$$

$$\Rightarrow g(E) = \frac{2\pi V}{\hbar^3} (2m)^{3/2} E^{1/2} \quad \leftarrow \text{density of states}$$

★ density of states represents the increase in number of states in which a particle can exist when the energy of the particle is increased by dE .

$$\text{i.e. } \frac{dN}{dE} = g(E)$$

$$dN = g(E) dE$$

dE corresponding to dk

For change in dk , we have change in volume dV in state space.

Every state occupies $\left(\frac{\pi}{L}\right)^3$ \times $\left(\frac{\pi}{L}\right)^3$ \times $\left(\frac{\pi}{L}\right)^3$ volume

$$\Rightarrow dV = \frac{dV}{\left(\frac{\pi^3}{L^3}\right)} = \frac{\frac{1}{8} \times 4\pi k^2 dk}{\left(\frac{\pi^3}{L^3}\right)}$$

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

$$dk = \sqrt{\frac{2m}{\hbar^2}} \frac{dE}{2\sqrt{E}}$$

$$\Rightarrow dN = \frac{\frac{1}{8} \times 4\pi \frac{2m}{\hbar^2} E \left(\frac{2m}{\hbar^2}\right)^{\frac{1}{2}} \frac{1}{2} (E)^{-\frac{1}{2}} dE}{\left(\frac{\pi^3}{V}\right)}$$

$$= \frac{\frac{\pi}{4} \frac{(2m)^{3/2}}{\hbar^3} \sqrt{E}}{\frac{\pi^3}{V}} dE$$

$$= \frac{\pi}{4} \times \frac{V}{\pi^3} \times \frac{(2m)^{3/2}}{\hbar^3} \times 8\pi^3 \times \sqrt{E} dE$$

\Rightarrow

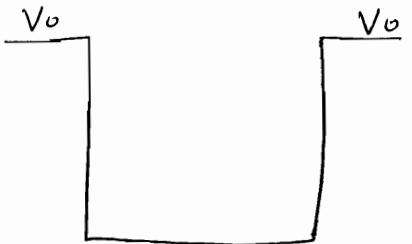
$$\boxed{\left(\frac{dN}{dE}\right) = 2\pi V \frac{(2m)^{3/2}}{\hbar^3} \sqrt{E}}$$

Quantum Mechanics (7)

13/02/2012

- We have done ~~step~~ as well as ~~infinite~~ Potential well (1-d as well as 3-d) problems.

Finite Well Problem



if V_0 is finite \Rightarrow Finite Well (Potential Problem)
(on both sides) or

(on 1 side) Step Potential Problem

if $V_0 \rightarrow \infty \Rightarrow$ Infinite Well Problem.

- We can also write,
by taking other reference point.

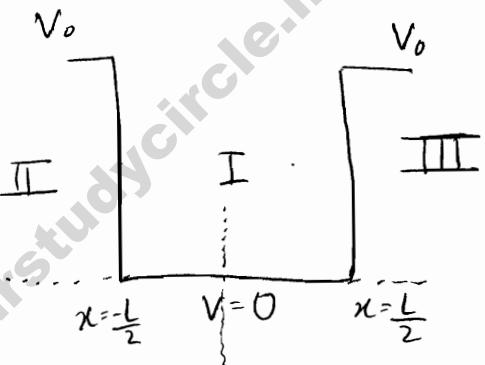
as

$$\begin{cases} |x| < \frac{L}{2}, & V = 0 \\ |x| > \frac{L}{2}, & V = V_0 \end{cases}$$

or

$$|x| < \frac{L}{2}, \quad V = -V_0$$

$$|x| > \frac{L}{2}, \quad V = 0$$



since reference axis is between, we will get closed form of solutions.

now
we will
solve for
this

We can solve
corresponding
solutions....

Step I

For I : $\frac{d^2\psi_1}{dx^2} + \frac{2m(E)}{\hbar^2} \psi_1 = 0 \quad (V=0)$

$$\psi_1 = A \cos k_1 x + B \sin k_1 x$$

closed
form
solutions

For II

$$x < \frac{L}{2}$$

$$\frac{d^2\psi_2}{dx^2} + \frac{2m}{\hbar^2} (E - V_0) \psi_2 = 0 \quad (E > V_0)$$

$$\rightarrow \psi_2 = C e^{ik_2 x} \quad (\text{Note that } x < 0)$$

←

For III

$$x > \frac{L}{2}$$

$$\frac{d^2\psi_3}{dx^2} + \frac{2m}{\hbar^2} (E - V_0) \psi_3 = 0$$

$$\psi_3 = D e^{ik_3 x} \quad (\text{Note that } x > 0)$$

→

But we are more interested in $E < V_0$ or i.e. Particle is "trapped" inside Potential Well V_0 .

Region II $\frac{d^2\psi_2}{dx^2} - \frac{2m}{\hbar^2} (V_0 - E) \psi_2 = 0$

$$\psi_2 = C e^{k_2 x} \quad (x < 0)$$

Region III

$$\frac{d^2\psi_3}{dx^2} + \frac{2m}{\hbar^2} (V_0 - E) \psi_3 = 0$$

$$\psi_3 = D e^{-k_3 x}$$

Solution in Central Region is Trigonometric
 Solution in outer regions is Exponentially decreasing.

$x > 0$ and $y > 0$

Step 3

Multiply symmetric solution by $\left(\frac{L}{2}\right)$

$$k_1 \frac{L}{2} \tan k_1 \frac{L}{2} = k_2 \frac{L}{2}$$

\downarrow \downarrow

$$x \tan x = y$$

$$x = \frac{\sqrt{2mE}}{\hbar} \frac{L}{2}$$

$$y = \frac{\sqrt{2m(V_0 - E)}}{\hbar} \frac{L}{2}$$

Asymmetric solution

$$\tan(90 + \theta) = -\cot \theta$$

$$-x \cot x = y$$

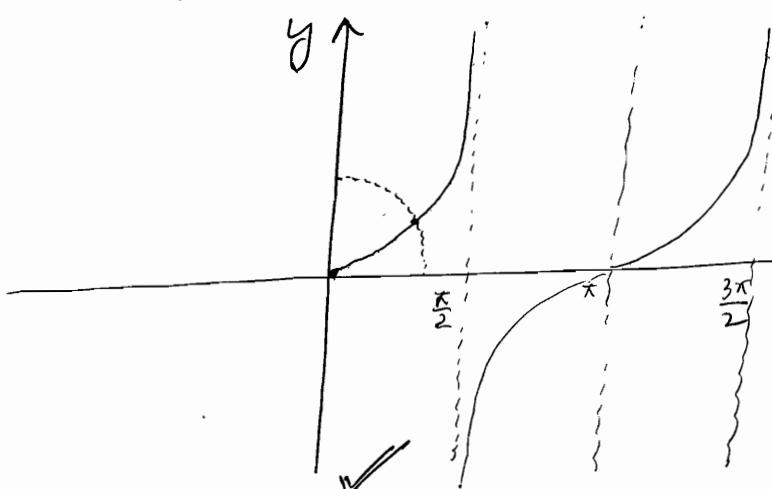
$$x \tan\left(\frac{\pi}{2} + x\right) = y$$

Also note $x^2 + y^2 = \frac{2m}{\hbar^2} \frac{L^2}{4} V_0 = \left(\frac{m V_0 L^2}{2\hbar^2}\right) = R^2$ (say)

Now we have 2 equations and 2 variables

$V_0 L^2$: strength parameter of well.

$$x^2 + y^2 = \left(\frac{m}{2\hbar^2}\right) V_0 L^2$$



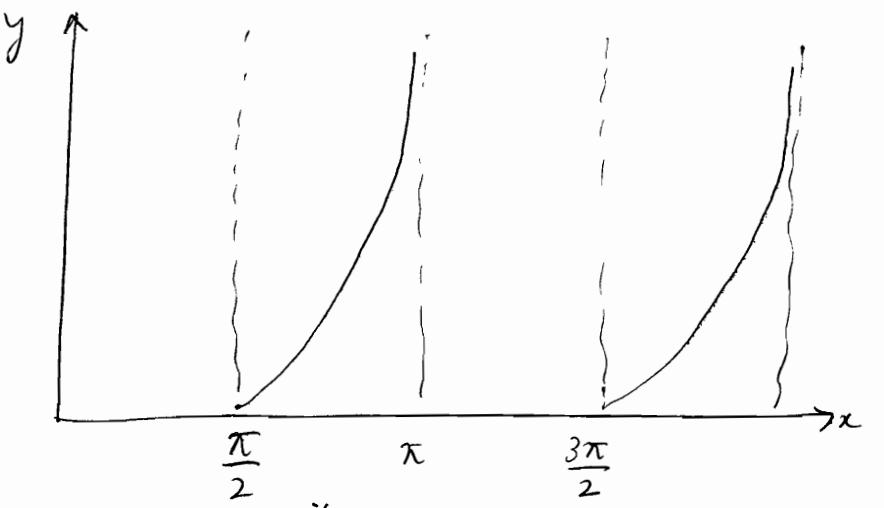
if $R < \frac{\pi}{2}$

$$\text{i.e. } V_0 L^2 < \left(\frac{\pi^2 \hbar^2}{2m}\right)$$

\Rightarrow Only 1 particular value of E is obtained:

a symmetric solution

we are interested only in this region



$$y = x \cot x$$

① ground state
it always symmetric
solution it'll be!!

If $R < \frac{\pi}{2}$,
no asymmetric solution

| <u>Possible</u> | <u>Possible</u> |
|-------------------------------|-------------------------------------|
| <u>Symmetric</u> | <u>Asymmetric or Anti-symmetric</u> |
| $\frac{R}{L} < \frac{\pi}{2}$ | 1 |
| $= \frac{\pi}{2}$ | 1 |
| $\frac{\pi}{2} < R < \pi$ | 1 |
| $\pi \leq R < \frac{3\pi}{2}$ | 2 |
| | 0 |
| | 1 |
| | 1 |
| | 1 |

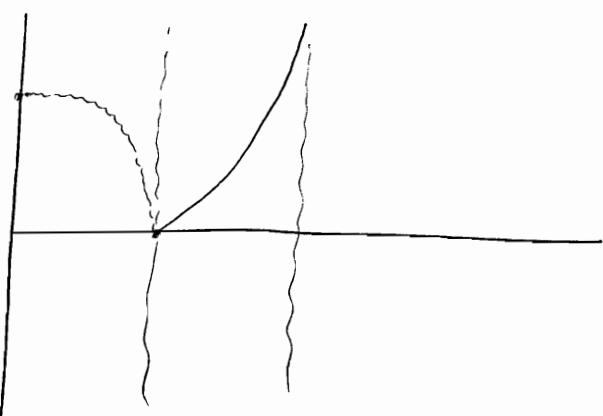
We will write as

$$\pi^2 < R^2 < \frac{9\pi^2}{4}$$

$$\text{i.e. for, } \frac{2\pi^2 h^2}{m} < V_0 L^2 < \frac{18\pi^2 h^2}{m}$$

we have 3 possible states.

2 symmetric and 1 anti-symmetric



$$R \geq \frac{\pi}{2}$$

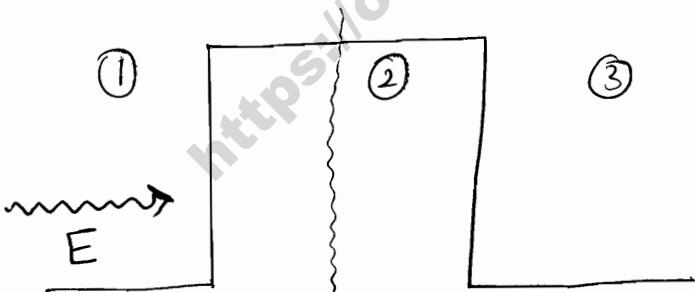
$$R^2 \geq \frac{\pi^2}{4}$$

$$\frac{2m}{\hbar^2} V_0 a^2 \geq \frac{\pi^2}{4}$$

$$\Rightarrow V_0 a^2 \geq \left(\frac{\hbar^2 \pi^2}{8m} \right)$$

RECTANGULAR BARRIER

- Opposite of Finite Well or 2-step Potential Problem
- Barrier is always of finite height.



$$x < -\frac{L}{2}, \quad V=0$$

$$x > \frac{L}{2}, \quad V=0$$

$$-\frac{L}{2} < x < \frac{L}{2} : \quad V = V_0$$

$$R = \left(\frac{J_r}{J_i} \right) \quad T = \left(\frac{J_t}{J_i} \right)$$

Step I : Setting of Schrodinger Equations

$$\textcircled{1} \quad \frac{d^2\psi_1}{dx^2} + \frac{2mE}{\hbar^2} \psi_1 = 0$$

$$\psi_1 = \underline{A e^{ik_1 x}} + \underline{B e^{-ik_1 x}}$$

$$R = \frac{|B|^2}{|A|^2}$$

as we did for finite step potential

$$\textcircled{3} \quad \frac{d^2\psi_3}{dx^2} + \frac{2mE}{\hbar^2} \psi_3 = 0$$

$$\psi_3 = \underline{F e^{ik_3 x}}$$

[Note that no returning wave]

$$T = \frac{|F|^2}{|A|^2}$$

\textcircled{2} Quantum Mechanically, important case is $E < V_0$
 Particle crossing, if $E < V_0$, solution is called Tunneling Phenomenon.

$$\underline{E > V_0} \quad \frac{d^2\psi_2}{dx^2} + \frac{2m}{\hbar^2} (E - V_0) \psi_2 = 0$$

$$\psi_2 = C e^{ik_2 x} + D e^{-ik_2 x}$$

For E < V_o

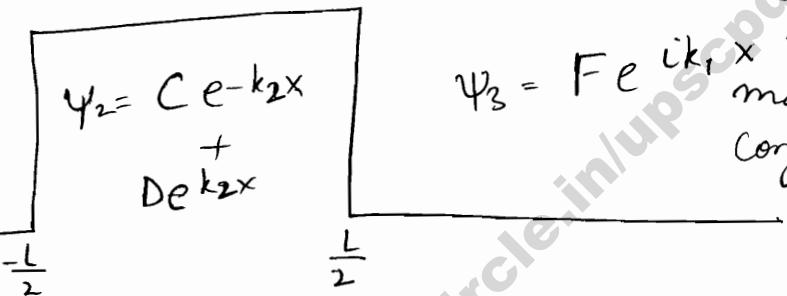
$$\frac{d^2\psi_2}{dx^2} - \frac{2m}{\hbar^2} (V_o - E) \psi_2 = 0$$

$$\Rightarrow \psi_2 = C e^{-k_2 x} + D e^{k_2 x}$$

[Note that nothing is 0 as x is finite)

Step II Boundary Conditions

$$\psi = A e^{ik_1 x} + B e^{-ik_1 x}$$



* do not use alphabets like 'E' or 'H' or 'J' etc. for naming. They may lead to confusion.

$$\psi_1 = \psi_2$$

$$\frac{d\psi_1}{dx} = \frac{d\psi_2}{dx}$$

$$A e^{ik_1 \frac{L}{2}} + B e^{-ik_1 \frac{L}{2}} =$$
$$C e^{-k_2 \frac{L}{2}} + D e^{k_2 \frac{L}{2}}$$

Solve for (B/A)

$$\left(\frac{F}{A}\right)$$

$$k_1 A e^{ik_1 \frac{L}{2}} - k_1 B e^{-ik_1 \frac{L}{2}}$$

$$= -C k_1 e^{-k_1 \frac{L}{2}} + k_1 D e^{k_1 \frac{L}{2}}$$

$$\psi_2 = \psi_3$$

$$\frac{d\psi_2}{dx} = \frac{d\psi_3}{dx}$$

—

—

By solving 4 equations in terms of A, we get,

(very rigorous algebra)

$$\approx \frac{16 V_0^2}{E(V_0 - E)} \left[\frac{e^{2x}}{4} + \frac{e^{-2x}}{4} + \frac{1}{2} \right]$$

~~\rightarrow~~

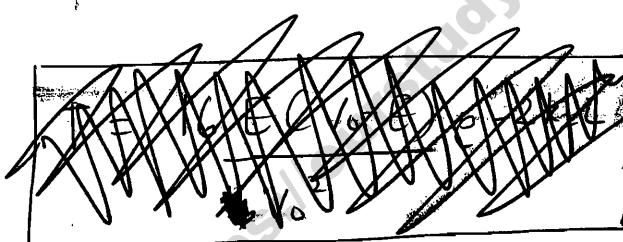
$$\frac{1}{T} = 1 + \frac{V_0^2}{4E(V_0 - E)} \sinh^2(k_2 L) \quad \text{neglect}$$

~~$x \text{ is large}$~~

$$\Rightarrow \frac{1}{T} = \frac{V_0^2}{4E(V_0 - E)} e^{2x} \quad \left(\frac{e^{2x}}{4} \right)$$

$$\Rightarrow \frac{1}{T} = \frac{V_0^2}{16 E(V_0 - E)} e^{2x}$$

~~\rightarrow~~



Formula
on
next page

Note that T is not zero here even if classically forbidden zone.

- Q) An α particle of energy 8 MeV is trapped in nucleus Potential Well of 35 MeV. Find out chance of crossing nucleus (i.e. transmission Coefficient)

$$R_{\text{nucleus}} = 10^{-15} \text{ m}$$

$$m_\alpha = 4 \times 1.66 \times 10^{-27} \text{ kg}$$

This problem is called Quantum Mechanical Tunneling.

$$\frac{16 \cdot 8 \cdot 27}{(35)^2} e^{-2 \sqrt{\frac{2m \cdot 27}{\hbar^2}} \cdot 10^{-15}}$$

~~40~~

Matter of fact is that α particle makes 10^{40} attempts and comes out of nucleus ... observed fact.

$$\phi = k \frac{\hbar}{\Delta p} = \sqrt{2m(V_0 - E)}$$

$$\Delta p = \sqrt{2m(V_0 - E)}$$

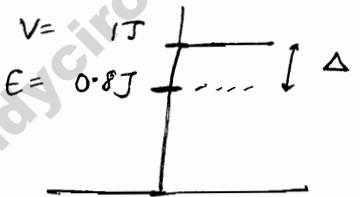
$$\Delta x = \frac{\hbar}{2\sqrt{2m(V_0 - E)}}$$

$$\Delta E = \frac{(\Delta p)^2}{2m} = (V_0 - E)$$

$$\Rightarrow V_0 = E + \Delta E.$$

$$T = E - V_0 = -\Delta E$$

Error can be in both ways
 \rightarrow what we have said $E < V_0$
 there can be uncertainty in measurement of E and V .



Δ is error in measurement of E

- (*) Note that in Energy Uncertainty Principle, there is no inequality but rather $\Delta E \Delta t \approx \hbar$
- If $\Delta = -(V_0 - E)$
 $\Rightarrow E$ is just equal to V
 Hence, Particle can escape.

$$\boxed{V_0 > E} T = \frac{4E(V_0 - E)}{4E(V_0 - E) + V_0^2 \sinh^2(rL)} \approx e^{-2rL}$$

$$\boxed{V_0 < E} T = \frac{4E(E - V_0)}{4E(E - V_0) + V_0^2 \sin^2(rL)} \approx e^{-2rL}$$

$$R = 1 - T$$

Approximation if $rL > 5$

- (*) 4 examples of tunneling \rightarrow
- ① α -decay
 - ② Field emission

- ③ Tunneling b/w metals
Scanning Tunneling Microscope
- ④ Nuclear Fusion

Quantum Mechanics (8)

14/02/2012

Simple Harmonic Oscillator

Simple implies 1-d motion.

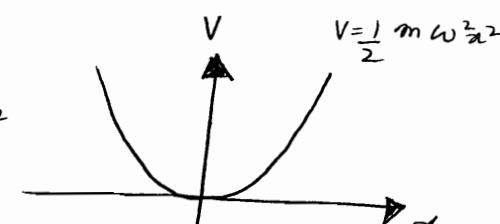
$$F \propto -x$$

$$F = -kx$$

$$V = -\int F \cdot dx = \frac{1}{2} kx^2 = \frac{1}{2} m\omega^2 x^2$$

$$E = \frac{p^2}{2m} + \frac{1}{2} m\omega^2 x^2$$

$$(T) \quad (V)$$



Parabolic Potential Well

Classically, it can have any value of energy including 0.

$$\left[\text{as } A \rightarrow 0, \frac{1}{2} k A^2 \rightarrow 0 \right]$$

But we need to measure Energy Quantum Mechanically.

$$\text{i.e. } H\psi = E\psi$$

$$\Rightarrow \frac{-\hbar^2}{2m} \frac{d^2\psi}{dx^2} + V\psi = E\psi$$

$$\Rightarrow \frac{d^2\psi}{dx^2} + \frac{2m(E-V)}{\hbar^2} \psi = 0$$

$$\Rightarrow \boxed{\frac{d^2\psi}{dx^2} + \left[\frac{2m(E)}{\hbar^2} - \frac{m^2\omega^2 x^2}{\hbar^2} \right] \psi = 0} \quad \text{--- (1)}$$

Note that till now, V was const. , hence easy differential equations.

Now the solution of differential equation has become complex.

Better solution is obtained by variation of parameter,

let the solution be

$$\underline{\text{Step III}} \quad \Psi_1(y) = C u(y) \Psi_0(y)$$

1st iteration

where

$$u_n(y) = \sum_{n=0}^{\infty} a_n y^n \quad \text{i.e. } n\text{th degree polynomial in } y$$

This solution should satisfy ④

Calculating,

$$\frac{dy}{dy} = -C y e^{-(\frac{y^2}{2})} u(y) + C e^{-\frac{y^2}{2}} \frac{(du)}{dy}$$

$$\frac{d^2y}{dy^2} = -C e^{-\frac{y^2}{2}} + C y^2 e^{-\frac{y^2}{2}}$$

$$+ C e^{-\frac{y^2}{2}} \frac{d^2u}{dy^2} + y C \left(\frac{du}{dy} \right) e^{-\frac{y^2}{2}}$$

While deriving
write $u(y)$ or just
 u instead of
 $u(y)$ otherwise
confusion can
occur !!

$$\frac{d^2y}{dy^2} = C e^{-\frac{y^2}{2}} \left[\frac{d^2u}{dy^2} - 2y \frac{du}{dy} + (y^2 - 1) u \right]$$

④ Also no need of
C while deriving

Hence Putting in ④, we get

$$C e^{-\frac{y^2}{2}} \left[\frac{d^2u}{dy^2} - 2y \frac{du}{dy} + (y^2 - 1) u + \frac{2E}{\hbar w} u - \frac{y^2 u}{\hbar w} \right] = 0$$

$$\Rightarrow C e^{-\frac{y^2}{2}} \left[\frac{d^2u}{dy^2} - 2y \left(\frac{du}{dy} \right) + \left(\frac{2E}{\hbar w} - 1 \right) u \right] = 0$$

$C \neq 0$, $e^{-\frac{y^2}{2}}$ cannot be 0

$$\Rightarrow \boxed{\frac{d^2u}{dy^2} - 2y\left(\frac{du}{dy}\right) + \left(\frac{2E}{\hbar\omega} - 1\right) u = 0} \quad - (5)$$

if the number is "2n", then
the differential equation is Hermite's
Differential Equation.

If that is so, then solutions are Hermite's Polynomials.

i.e. $P_n = (-1)^n e^{y^2} \frac{d^n (e^{-y^2})}{dy^n}$

Step 5

Let $\frac{2E_n}{\hbar\omega} - 1 = 2n$

$$\frac{2E_n}{\hbar\omega} = (2n+1) \Rightarrow E_n = \left(n + \frac{1}{2}\right) \hbar\omega$$

$$\Rightarrow \psi_n(y) = C_n U_n(y) e^{-\frac{y^2}{2}}$$

Step 4 Power series solution of (5) i.e.

$$\frac{d^2u}{dy^2} - 2y\left(\frac{du}{dy}\right) + \left(\frac{2E}{\hbar\omega} - 1\right) u = 0$$

$$U_n(y) = \sum_0^{\infty} a_n y^n = a_0 + a_1 y + a_2 y^2 + \dots + a_n y^n + \dots$$

$$\text{as } n \rightarrow \infty, a_n \rightarrow 0$$

i.e. every subsequent coefficient is lesser than previous coefficient. hence $\frac{a_{n+2}}{a_n} \rightarrow 0$

$$\frac{du}{dy} = \sum_{n=1}^{\infty} n a_n y^{n-1} = \sum_{n=0}^{\infty} n a_n y^{n-1} \quad [\text{as } @_{n=0} \text{ term=0}]$$

$$\frac{d^2 u}{dy^2} = \sum_{n=2}^{\infty} n(n-1) a_n y^{n-2} = \sum_{n=0}^{\infty} n(n-1) a_n y^{n-2}$$

Substituting in ⑤,

$$\sum_{n=0}^{\infty} n(n-1) a_n y^{n-2} - 2y \sum_{n=0}^{\infty} n a_n y^{n-1} + \left(\frac{2E}{\hbar\omega} - 1\right) \sum a_n y^n = 0$$

$$\uparrow \\ \text{Put } n' = \underline{n+2}$$

$$\sum_{n'=-2}^{\infty} (n'+2)(n'+1) a_{n'+2} y^{n'} - \sum 2n a_n y^n + \left(\frac{2E}{\hbar\omega} - 1\right) \sum a_n y^n = 0$$

$$= \sum_{n'=0}^{\infty} [\text{as } n'+2=0 @ n'=-2] \quad [\text{as } n'+1=0 @ n'=-1]$$

$$\sum_{n=0}^{\infty} \left[(n+2)(n+1) a_{n+2} + \left(\frac{2E}{\hbar\omega} - 1 - 2n\right) a_n \right] y^n = 0$$

Step 4
Now if it is true for $\forall n \Rightarrow y^n$ cannot be 0

$$\Rightarrow \frac{a_{n+2}}{a_n} = \frac{\left(2n+1 - \frac{2E_n}{\hbar\omega}\right)}{(n+2)(n+1)}$$

$$\frac{a_{n+2}}{a_n} = 0$$

(terminates)

Write P_n instead of u_n in final solution

In order that $u_n(y)$ does not diverge, it must be some power of $n \Rightarrow a_{n+2} = 0$

$$\Rightarrow n \text{ QR} \quad (2n+1) = \frac{2E}{\hbar\omega} \quad \Rightarrow$$

Condition $3+1 \text{ QR} !!$
 $\Rightarrow n \neq 0, 2 \text{ and } E \text{ is a valid value} !!$

$$E_n = \left(n + \frac{1}{2}\right) \hbar\omega$$

$$\Psi_n(y) = C_n u_n(y) e^{-\frac{y^2}{2}}$$

where $u_n(y)$ are hermite's polynomials

$$u_n(y) = \frac{(-1)^n}{\boxed{\text{[Redacted]}}} e^{-\frac{y^2}{2}} \frac{d^n}{dy^n} (e^{-\frac{y^2}{2}})$$

$$u_0(y) = 1$$

$$u_1(y) = 2y$$

$$u_2(y) = 4y^2 - 2$$

$$u_3(y) = 8y^3 - 12y$$

even
odd
even
odd
.

Ground state energy

$$\underline{n=0}$$

$$\psi_0(y) = C_0 u_0(y) e^{-\frac{y^2}{2}}$$

$$\psi_0(y) = C_0 \cdot 1 \cdot e^{-\frac{y^2}{2}} = C_0 e^{-\frac{(y^2)}{2}}$$

$$\boxed{E_0 = \left(\frac{\hbar\omega}{2}\right)} \quad \boxed{\psi_0(y) = C_0 e^{-\frac{y^2}{2}}} = C_0 e^{-\frac{m\omega x^2}{2\hbar}}$$

1st excited level

$$\underline{n=1}$$

$$u_1(y) = \frac{-1}{\boxed{\text{[Redacted]}}} e^{-\frac{y^2}{2}} \cdot e^{-\frac{y^2}{2}} = 2y$$

$$\Rightarrow \boxed{\psi_1(y) = 2C_1 y e^{-\frac{(y^2)}{2}}} = 2C_1 \sqrt{\frac{m\omega}{\hbar}} x e^{-\frac{m\omega x^2}{2\hbar}}$$

Note that C_n 's will be calculated using normalization, i.e.

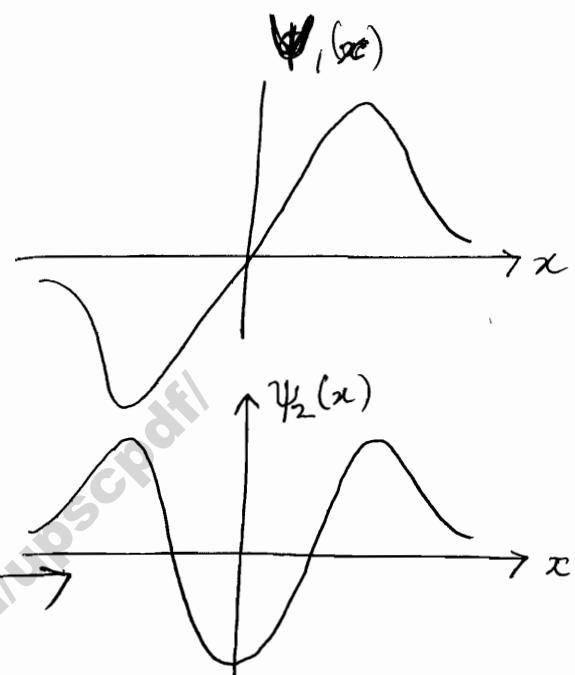
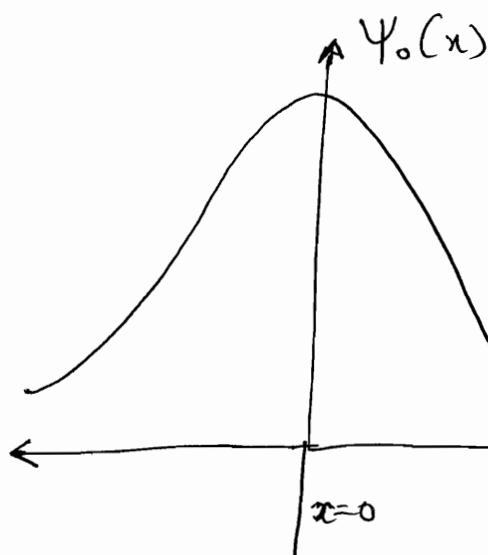
$$|\psi \psi^*| = 1$$

$$C_0^2 \int_{-\infty}^{\infty} e^{-\frac{m\omega x^2}{\hbar}} dx = 1 \quad \Rightarrow \quad C_0 = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}}$$

$$\Rightarrow C_0^2 \sqrt{\frac{\pi\hbar}{m\omega}} = 1 \quad \checkmark$$

$$\Rightarrow \Psi_0(x) = \left(\frac{m\omega}{\pi\hbar} \right)^{\frac{1}{4}} e^{-\frac{m\omega}{2\hbar}x^2}$$

$$E_0 = \frac{1}{2} \hbar \omega$$



Gaussian Wave Function

Probability will also be gaussian !!



Zero Point Energy : $n=0$ $E_0 = \frac{1}{2} \hbar \omega$

Commensurate with Heisenberg Uncertainty Principle

✓ Classically, energy can have any values while

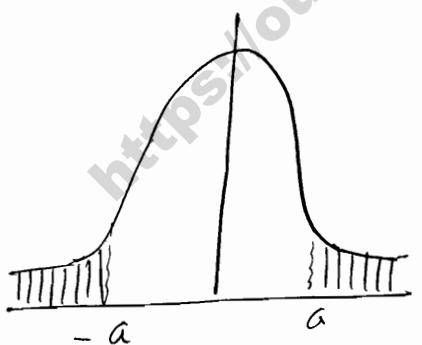
Quantum Oscillator can have ~~any~~ only discrete values of energy $(n+\frac{1}{2})\hbar\omega$ \Rightarrow Note that quantums are so small that it appears almost continuous.....

✓ Classical Oscillator can have minimum energy 0. while

Quantum Oscillator can have minimum energy as $(\frac{\hbar\omega}{2})$ commensurate with H.U.P.

✓ Classically, Oscillator goes between $\pm a$ while

Quantum Mechanically, Oscillator can move from $[-\infty, +\infty]$ e.g. in ground state 16% chance of it being located outside $\pm a$.



$$\psi_0^2(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{2}} e^{-\frac{m\omega}{\hbar}x^2}$$

$$\int_{-\infty}^{\infty} \psi_0^2(x) dx = 1$$

$|x| > a$: Classically Forbidden Region
 $|x| < a$: Classically allowed region

$$P_{|x| < a} = \int_{-a}^a \psi_0^2(x) dx = \sqrt{\frac{m\omega}{\pi\hbar}} \int_{-a}^a e^{-\frac{m\omega x^2}{\hbar}} dx - ⑥$$

$$P_{|x| > a} = 1 - \int_{-a}^a \psi_0^2(x) dx = 1 - 0.84 \\ \approx 16\%$$

To calculate ⑥

$$\frac{1}{2} m \omega^2 a^2 = \left(\frac{\hbar \omega}{2} \right)$$

[classically, Total Energy = Potential Energy]

$$\Rightarrow a = \sqrt{\frac{\hbar}{m\omega}}$$

$$\Rightarrow P_{|x| < a} = \sqrt{\frac{m\omega}{\pi\hbar}} \int_{-\sqrt{\frac{\hbar}{m\omega}}}^{\sqrt{\frac{\hbar}{m\omega}}} e^{-\frac{m\omega x^2}{\hbar}} dx$$

$$\text{Put } \sqrt{\frac{m\omega}{\hbar}} x = t \Rightarrow \sqrt{\frac{m\omega}{\hbar}} dx = dt$$

$$\Rightarrow P_{|x| < a} = \frac{1}{\sqrt{\pi}} \int_{-1}^1 e^{-t^2} dt = \frac{2}{\sqrt{\pi}} \int_0^1 e^{-t^2} dt$$

It is an "Error Function".... It cannot be integrated
We can have only approximate values.

$$= \frac{1}{\sqrt{\pi}} \int_1^1 \left[1 - t^2 + \frac{t^4}{L^2} + \dots \right] dt$$

$$= \frac{1}{\sqrt{\pi}} \left[\left[1 - \frac{t^3}{3} + \frac{t^5}{10} \right] \right]_1^1$$

$$\approx 0.84$$

① To show that ψ is commensurate with Heisenberg Uncertainty Principle :

i.e. Show $\Delta x \Delta p_x \geq \left(\frac{\hbar}{2}\right)$

Also $\langle T \rangle = \frac{\langle p_x^2 \rangle}{2m} = \underline{\underline{\left(\frac{\hbar\omega}{4}\right)}}$

$$\langle V \rangle = \frac{1}{2} m \omega^2 \langle x^2 \rangle = \underline{\underline{\left(\frac{1}{4}(\hbar\omega)\right)}}$$

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

$$\langle x \rangle = \int \psi^* x \psi dx = \left(\frac{m\omega}{\pi\hbar} \right)^{\frac{1}{2}} \int_0^\infty x e^{-\frac{m\omega}{\hbar}x^2} dx$$

$$\Delta p = \sqrt{\langle p_x^2 \rangle - \langle p_x \rangle^2} = 0 \quad [\text{odd function}]$$

$$\langle p_x \rangle = \int_{-\infty}^{\infty} \psi^* i\hbar \frac{\partial}{\partial x} \psi dx = 0$$

[Odd function]

$$\langle x^2 \rangle = \left(\frac{m\omega}{\pi\hbar} \right)^{\frac{1}{2}} \int_{-\infty}^{\infty} x^2 e^{-\frac{m\omega}{\hbar}x^2} dx$$

$$= \left(\frac{m\omega}{\pi\hbar} \right)^{\frac{1}{2}} 2 \int_0^\infty x^2 e^{-\left(\frac{m\omega}{\hbar}\right)x^2} dx$$

$\langle x \rangle : 0$ easy
 $\langle x^2 \rangle : \checkmark$ easy
 $\langle p_x \rangle : 0$ directly
 $\langle p_x^2 \rangle : \text{use } T \text{ easy}$

$$= 2 \left(\frac{m\omega}{\pi\hbar} \right)^{\frac{1}{2}} \cdot \frac{1}{2 \left(\frac{m\omega}{\hbar} \right)^{\frac{3}{2}}} \cdot \sqrt{\frac{3}{2}}$$

$$= \frac{1}{2} \left(\frac{\hbar}{m\omega} \right) \Rightarrow \Delta p_x$$

$$= \sqrt{\frac{\hbar}{2m\omega}} \sqrt{\frac{\hbar m\omega}{2}} = \left(\frac{\hbar}{2} \right)$$

$$\langle p_x^2 \rangle = \frac{\hbar m\omega}{2}$$

$$\begin{aligned} & \left[\alpha = \frac{m\omega}{\hbar} \right] \\ & -\hbar^2 \left(\frac{\alpha}{\pi} \right)^{\frac{1}{2}} \int_{-\infty}^{\infty} e^{-\frac{\alpha x^2}{2}} \frac{\partial^2 (e^{-\frac{\alpha x^2}{2}})}{\partial x^2} dx \\ & = -2\hbar^2 \sqrt{\frac{\alpha}{\pi}} \int_{-\infty}^{\infty} \alpha^2 x^2 e^{-\alpha x^2} - \alpha e^{-\alpha x^2} dx = -2\hbar^2 \sqrt{\alpha} \left[\frac{\sqrt{\alpha}}{4} - \frac{\sqrt{\alpha}}{2} \right] = \frac{\hbar^2 \alpha}{2} = \frac{\hbar m\omega}{2} \end{aligned}$$

Matrix Representation

Refer to lecture 11

$$H\psi = E\psi$$

$$\Rightarrow H = \left(n + \frac{1}{2} \right) \hbar\omega [I]_n$$

$$\Rightarrow H = \begin{bmatrix} \frac{1}{2}\hbar\omega & 0 & 0 & 0 & \dots & \\ 0 & \frac{3}{2}\hbar\omega & 0 & 0 & \dots & \\ 0 & 0 & \frac{5}{2}\hbar\omega & 0 & \dots & \\ \dots & \dots & \dots & \dots & \dots & \\ 0 & 0 & 0 & 0 & \dots & \\ & & & & & 0 \left(n + \frac{1}{2} \right) \hbar\omega \end{bmatrix}$$

$$A [I_n] \begin{bmatrix} \psi_n \\ \vdots \\ \psi_1 \end{bmatrix} = \begin{bmatrix} \psi_n \\ \vdots \\ \psi_1 \end{bmatrix}$$

$n \times n \quad n \times 1$

Pure Number $n \times 1$

$$\psi(x) = \frac{1}{\sqrt{3}} \left\{ \psi_0(x) + \sqrt{2} \psi_1(x) + \sqrt{2} \psi_2(x) \right\}$$

$$\langle \psi | \psi \rangle = 1 = \sum a_i^2$$

$$p_i = |\langle \phi_i | \psi \rangle|^2 = (a_i)^2 : \text{Probability of state } i$$

$$\begin{aligned}
 \langle E \rangle &= \langle \psi | H | \psi \rangle \\
 &= \frac{1}{5} \langle \psi_0 | H | \psi_0 \rangle + \frac{2}{5} \langle \psi_1 | H | \psi_1 \rangle \\
 &\quad + \frac{2}{5} \langle \psi_2 | H | \psi_2 \rangle \\
 &= \frac{1}{5} \times \left(\frac{5\hbar\omega}{2} \right) + \frac{2}{5} \times \left(\frac{3\hbar\omega}{2} \right) + \frac{2}{5} \left(\frac{5\hbar\omega}{2} \right) \\
 &= \frac{(1+6+10)\hbar\omega}{10} = \underline{\underline{\frac{17}{10}\hbar\omega}}
 \end{aligned}$$

Harmonic Oscillator Problem is done !!

- ★ do not go into double derivative. To find out $\langle p_x^2 \rangle$ always use $\langle T \rangle$.

Advanced Quantum Mechanics



Or

Quantum Mechanics (II)

Angular Momentum Problem

We know, dynamical variable 'a' represented by Hermitian Operator A

✓ s.t. $A\psi = a\psi$

✓ We also know representation of $A\psi$ as $a\psi$ in matrix form using $[I_n]$

$$\begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix} = a \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix}$$

✓ Also, $[A \ B] = FAB - BA$ $\begin{bmatrix} a & 0 \\ 0 & a \end{bmatrix} \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix} = a \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix}$

Now, $\vec{L} = \vec{J} = (\vec{r} \times \vec{p})$

$$\begin{aligned} &= \vec{r} \times -i\hbar \vec{\nabla} \\ &= -i\hbar \left[\vec{r} \times \vec{\nabla} \right] = -i\hbar \begin{bmatrix} i & j & k \\ x & y & z \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \end{bmatrix} \end{aligned}$$

$$\Rightarrow J_x = -i\hbar \left[y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right] = Y P_z - Z P_y$$

$$J_y = -i\hbar \left[z \frac{\partial}{\partial x} - x \frac{\partial}{\partial z} \right] = Z P_x - X P_z$$

$$J_z = -i\hbar \left[x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right] = X P_y - Y P_x$$

Note the cyclic order!!!

Quantum Mechanics (9)

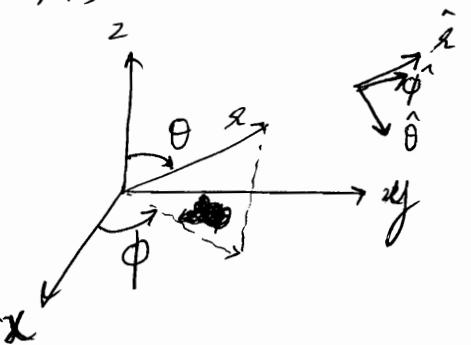
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We have studied

$$\vec{J} = \vec{r} \times \vec{p} = \vec{r} \times -i\hbar \vec{\nabla}$$

$$\Rightarrow \begin{cases} J_x = y P_z - z P_y \\ J_y = z P_x - x P_z \\ J_z = x P_y - y P_x \end{cases}$$

In (r, θ, ϕ) : spherical coordinates, we have



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

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

$$z = r \cos \theta$$

$\rightarrow \hat{i}, \hat{\theta}, \hat{\phi}$ are in the direction of increasing variables.

$[r, \theta, \phi]$ form a right handed triad

We know, in spherical coordinates,

$$\vec{\nabla} = \frac{\partial}{\partial r} \hat{r} + \frac{1}{r} \frac{\partial}{\partial \theta} \hat{\theta} + \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} \hat{\phi}$$

$$\vec{L} = -i\hbar \begin{vmatrix} \hat{r} & \hat{\theta} & \hat{\phi} \\ r & 0 & 0 \\ \frac{\partial}{\partial r} & \frac{1}{r} \frac{\partial}{\partial \theta} & \frac{1}{r \sin \theta} \frac{\partial}{\partial \phi} \end{vmatrix}$$

$\vec{r} = r \hat{r}$
[of course \vec{r} has no component in $\hat{\theta}$ or $\hat{\phi}$]

$$= -i\hbar \left[\left[-\frac{1}{\sin \theta} \frac{\partial}{\partial \phi} \right] \hat{\theta} + \left[\frac{\partial}{\partial \theta} \right] \hat{\phi} \right]$$

Note that no 'i' term in \vec{L}

\rightarrow Note that these are just directions ... operator will operate upon ψ or other function.....

$$\vec{r} = x \hat{i} + y \hat{j} + z \hat{k}$$

$$= r \sin\theta \cos\phi \hat{i} + r \sin\theta \sin\phi \hat{j} + r \cos\theta \hat{k}$$

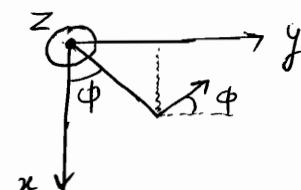
$$\hat{r} = \underline{\sin\theta \cos\phi \hat{i} + \sin\theta \sin\phi \hat{j} + \cos\theta \hat{k}}$$

$$\hat{\theta} = \underline{\sin(90+\theta) \cos\phi \hat{i} + \sin(90+\theta) \sin\phi \hat{j} + \cos(90+\theta) \hat{k}}$$

$$= \underline{\cos\theta \cos\phi \hat{i} + \cos\theta \sin\phi \hat{j} - \sin\theta \hat{k}}$$

$$\hat{\phi} = \hat{r} \times \hat{\theta}$$

$$= \underline{-\sin\phi \hat{i} + \cos\phi \hat{j}} \quad [\text{See and write}]$$



Hence, we can write

$$\vec{L} = -i\hbar \left[\frac{\partial}{\partial \theta} \left\{ -\sin\phi \hat{i} + \cos\phi \hat{j} \right\} \right]$$

$$- \frac{1}{\sin\theta} \frac{\partial}{\partial \phi} \left\{ \cos\theta \cos\phi \hat{i} + \cos\theta \sin\phi \hat{j} - \sin\theta \hat{k} \right\}$$

Note that
these are
not
operating on
directions

$$= -i\hbar \left[\left\{ -\sin\phi \frac{\partial}{\partial \theta} - \frac{1}{\sin\theta} \cos\theta \cos\phi \frac{\partial}{\partial \phi} \right\} \hat{i} \right.$$

$$+ \left\{ \cos\phi \frac{\partial}{\partial \theta} - \frac{\cos\theta \sin\phi}{\sin\theta} \frac{\partial}{\partial \phi} \right\} \hat{j}$$

$$+ \left\{ \frac{\partial}{\partial \phi} \right\} \hat{k}$$

]

$$L_x = -i\hbar \left[-\sin\phi \frac{\partial}{\partial\theta} - \cot\theta \cos\phi \frac{\partial}{\partial\phi} \right]$$

$$L_y = -i\hbar \left[\cos\phi \frac{\partial}{\partial\theta} - \cot\theta \sin\phi \frac{\partial}{\partial\phi} \right]$$

$$L_z = -i\hbar \left[\frac{\partial}{\partial\phi} \right]$$

★ L Operator in spherical coordinates

$$\vec{L} \cdot \vec{L} = L_x^2 + L_y^2 + L_z^2$$

$$\Rightarrow L^2 = -\hbar^2 \left[\left(\frac{1}{r^2} \frac{\partial}{\partial r} \right) \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin^2\theta} \frac{\partial^2}{\partial\phi^2} \right]$$

We know

① Note that they are operators and not numbers

$$L_x^2 = L_x (L_x)$$

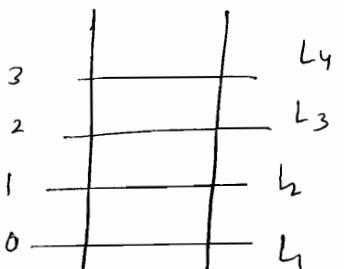
$$\begin{aligned} \nabla^2 &= \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin^2\theta} \frac{\partial^2}{\partial\phi^2} + \frac{1}{r^2 \sin\theta} \frac{\partial}{\partial\theta} \left(\sin\theta \frac{\partial}{\partial\theta} \right) \\ \text{Laplacean} &= \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2}{\partial\phi^2} \end{aligned}$$

$$L^2 = \hbar^2 r^2 \left[\nabla^2 - \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) \right]$$

$$L_x \pm iL_y = L_{\pm}$$

L_+ Operator takes the angular momentum to next quantized level.

L_- operator takes it 1 level below.



→ Quantum Mechanical values of $L \Rightarrow$ Quantized steps i.e. Particle in particular states

$$\left\{ L_{\pm} = \pm \hbar e^{\pm i\phi} \left[\frac{\partial}{\partial \theta} \pm i \cot \theta \frac{\partial}{\partial \phi} \right] \right\} \checkmark$$

Note that we can write,

$$L_x \Psi(r, \theta, \phi) = \lambda \Psi(r, \theta, \phi)$$

we can write $\Psi(r, \theta, \phi) = R(r) Y(\theta, \phi)$ [L has no dependency on r]

$$\Rightarrow L_x Y(\theta, \phi) = \lambda Y(\theta, \phi)$$

[L_x is independent of r]

If I want λ to be pure number,

$$\Rightarrow L_x Y(\theta, \phi) = \lambda \hbar Y(\theta, \phi)$$

Similarly,

$$L^2 Y(\theta, \phi) = \lambda \hbar^2 Y(\theta, \phi)$$

Angular Momentum Problem

Note that in order to determine L, we can determine L_z and only L_z . It will give unique values of L_x and L_y .

$$L_z = -i\hbar \frac{\partial}{\partial \phi}$$

Angular Momentum Problem

$$L^2 = -\hbar^2 \left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right]$$

$$L_z Y(\theta, \phi) = \lambda \hbar Y(\theta, \phi)$$

$$(i) L^2 \Psi(\theta, \phi) = \lambda \hbar^2 \Psi(\theta, \phi)$$

eigenvalue $L^2 = \lambda \hbar^2$

Angular Momentum

$$\Rightarrow |L| = \sqrt{\lambda} \hbar \quad \text{Magnitude Quantization}$$

$$(ii) L_z \Psi(\theta, \phi) = \lambda' \hbar \Psi(\theta, \phi) \quad \text{Space Quantization of Angular Momentum}$$

So our aim is to find λ , λ' and $\Psi(\theta, \phi)$

We can combine the 2 as,

$$[L^2, L_z] \left| \Psi(\theta, \phi) \right\rangle = 0 \quad \begin{aligned} &\checkmark \text{ Same eigenfunctions} \\ &\text{for both} \\ &\Rightarrow \text{commuting operators} \\ &\Rightarrow \text{commutator} = 0 \end{aligned}$$

$$[L^2, L_z] = 0$$

Simultaneous measurement is possible i.e. same Ψ .

$$\left. \begin{aligned} [L^2, L_x] &= 0 \\ [L^2, L_y] &= 0 \\ [L^2, L_z] &= 0 \end{aligned} \right\} \quad \begin{matrix} \checkmark \\ \text{any 1 of the 3} \end{matrix}$$

\rightarrow Note that simultaneous measurement of L^2 along with only 1 component is possible.

There will be error in measurement of other 2 components.

Let us start by solving the 2nd parts of Angular Momentum Problem.

$$L_2 Y(\theta, \phi) = \lambda' h Y(\theta, \phi)$$

$$-i\hbar \frac{\partial Y}{\partial \phi} = \lambda' h Y$$

$$\text{Put } \Theta(\theta) \Phi(\phi) = Y(\theta, \phi)$$

Solving it w/o separating the variables is WRONG !!

$$\Rightarrow \frac{\partial Y}{\partial \phi} = i\lambda' Y$$

$$\Rightarrow \cancel{\Theta(\theta)} \cdot \frac{\partial \Phi}{\partial \phi} = i\lambda' \cancel{\Theta(\theta)} \Phi(\phi)$$

$$\Rightarrow \boxed{\Phi = A e^{i\lambda' \phi}} \quad \text{--- (1)}$$

$$\frac{d\Phi}{d\phi} = i\lambda' \Phi$$

$$\Rightarrow \ln \Phi = i\lambda' \phi + A'$$

$$\Rightarrow \Phi = A e^{i\lambda' \phi}$$

$$\langle \Phi | \Phi \rangle = 1$$

$$\Rightarrow \int_0^{2\pi} |A|^2 e^{-i\lambda' \phi} e^{i\lambda' \phi} d\phi = 1$$

$$\Rightarrow |A|^2 \cdot 2\pi = 1$$

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

$$\text{Now we know } \Phi(\phi + 2\pi) = \Phi(\phi)$$

[Wave function must be single valued]

$$\Rightarrow \frac{1}{\sqrt{2\pi}} e^{i\lambda' (\phi + 2\pi)} = \frac{1}{\sqrt{2\pi}} e^{i\lambda' \phi}$$

$$\Rightarrow e^{i(2\pi \lambda')} = 1$$

$$\Rightarrow \cos(2\pi \lambda') = 1$$

$$\Rightarrow 2\pi \lambda' = 2n\pi$$

$$\boxed{\lambda' = n}$$

Hence λ' is an integer

$n=0, \pm 1, \pm 2, \pm 3, \dots$

From this part we got to know, that λ_z is the coefficient of $(i\phi)$ in exponent of $\Phi(\phi)$. we should have done this part after calculating $\Phi(\phi)$ done in Part II ...

$$\Rightarrow \boxed{L_z = m_e} \text{ Eigen Values of } L_z$$

Now solving 1st part of Angular Momentum Problem,

$$L^2 Y(\theta, \phi) = \lambda \hbar^2 Y(\theta, \phi)$$

$$\left[\frac{1}{\sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial}{\partial \theta} \right) + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \phi^2} \right] Y = -\lambda Y$$

$$\text{Put } Y(\theta, \phi) = \Theta(\theta) \Phi(\phi)$$

$$\Rightarrow \frac{\Theta}{\sin \theta} \frac{\partial}{\partial \theta} \left[\sin \theta \frac{\partial \Theta}{\partial \theta} \right] + \frac{\Theta}{\sin^2 \theta} \frac{d^2 \Phi}{d \phi^2} = -\lambda \Theta \Phi$$

divide by $\Theta \Phi$

$$\Rightarrow \frac{1}{\Theta \sin \theta} \frac{d}{d \theta} \left[\sin \theta \frac{d \Theta}{d \theta} \right] + \frac{1}{\sin^2 \theta \Phi} \frac{d^2 \Phi}{d \phi^2} = -\lambda$$

Multiply by $\sin^2 \theta$

$$\Rightarrow \frac{\sin \theta}{\Theta} \frac{d}{d \theta} \left[\sin \theta \frac{d \Theta}{d \theta} \right] + \lambda \sin^2 \theta = -\frac{1}{\Phi} \frac{d^2 \Phi}{d \phi^2} = m_e^2$$

(From eqn ① on last page)

LHS : $f(\theta)$

RHS : $f(\phi)$

Hence both are const.

\Rightarrow let them be ~~m_e^2~~ m_e^2

\rightarrow 2nd easier way is to 1st find eigenvalues & eigenfunctions of L_2 and then use them in L^2 as $[L^2, L_2] = 0 \Rightarrow$ they will have a complete set of common eigenfunctions.

$$-\frac{1}{\Phi} \frac{d^2 \Phi}{d\phi^2} = m_e^2$$

$$\Phi(\phi) = \frac{1}{\sqrt{2\pi}} e^{im_e \phi}$$
$$m_e = 0, \pm 1, \pm 2, \dots$$

$$\frac{\sin \theta}{\theta} \frac{d}{d\theta} \left(\sin \theta \frac{d\Theta}{d\theta} \right) + (\lambda \sin^2 \theta - m_e^2) = 0$$

~~a differential equation~~

let $\cos \theta = x$

$$-\sin \theta \frac{d\theta}{dx} = \frac{dx}{d\theta}$$

$$\frac{d}{d\theta} = \frac{d}{dx} \cdot \frac{dx}{d\theta} = -\sin \theta \frac{d}{dx}$$

First substitute and then do the derivative!! so that you do not have to derive for $(\frac{d^2}{d\theta^2})$

$$-\frac{\sin^2 \theta}{\theta} \frac{d}{dx} \left(-\sin \theta \frac{d\Theta}{dx} \right) + (\lambda \sin^2 \theta - m_e^2) = 0$$

$$\Rightarrow (1-x^2) \frac{d}{dx} \left((1-x^2) \frac{d\Theta}{dx} \right) + [\lambda(1-x^2) - m_e^2] \Theta = 0$$

$$\Rightarrow (1-x^2) \frac{d}{dx} \left((1-x^2) \frac{d\Theta}{dx} \right) + (\lambda(1-x^2) - m_e^2) \Theta = 0$$

differentiating &

dividing by $(1-x^2)$

{not necessary if not multiplied by $\sin \theta$, if doing in above manner}

$$(1-x^2) \frac{d^2\Theta}{dx^2} - 2x \frac{d\Theta}{dx} + \left[\lambda - \frac{m_e^2}{(1-x^2)} \right] \Theta = 0$$

It is Associated Legendre's Differential Equation

This is worked out by Power Series Method.

$\Theta(x)$ = Solutions are Associated Legendre's polynomials.

$$\Theta(x) = B P_e^{m_e}(x)$$

If $m_e = 0$ \Rightarrow Legendre's Differential Equation

$$(1-x^2) \frac{d^2\Theta}{dx^2} - 2x \frac{d\Theta}{dx} + \lambda \Theta = 0$$

Solution by Power Series Method

$$\text{Let } \Theta(x) = \sum_{l=0}^{\infty} a_l x^l = a_0 + a_1 x + a_2 x^2 + \dots$$

[Θ नहीं अपेक्षित है कि ये Power Series method

Note that $a_l \rightarrow 0$ as $x \rightarrow \infty$

$$\frac{d\Theta}{dx} = a_1 + 2a_2 x + \dots = \sum_{l=1}^{\infty} a_l l x^{l-1}$$

$$\frac{d^2\Theta}{dx^2} = 2a_2 + 3 \cdot 2 a_3 x + \dots = \sum_{l=2}^{\infty} a_l l(l-1) x^{l-2}$$

$$\Rightarrow \sum (1-x^2) a_l l(l-1) x^{l-2} - \sum 2x l a_l x^{l-1} \\ + \lambda \sum a_l x^l = 0$$

[do not touch the coefficient a_l while differentiating]

$$\Rightarrow \sum l(l-1) a_l x^{l-2} - \sum a_l l(l-1) x^l$$

$$- \sum 2l a_l x^l + \sum \lambda a_l x^l = 0$$

Put $l' = l+2$

$$\Rightarrow \sum (l'+2)(l'+1) a_{l'+2} x^l : 1^{\text{st}} \text{ term}$$

Now taking x^l : common

$$\Rightarrow \sum_{l=0}^{\infty} \left((l+2)(l+1) a_{l+2} - a_l l(l-1) - 2l a_l + \lambda a_l \right) x^l = 0$$

$$\Rightarrow (l+2)(l+1) a_{l+2} - [l(l+1) - \lambda] a_l = 0$$

$$\Rightarrow \frac{a_{l+2}}{a_l} = \frac{l(l+1) - \lambda}{(l+1)(l+2)}$$

Now Θ must converge otherwise x^∞ will diverge. \therefore must truncate
 $\frac{a_{l+2}}{a_l} \quad 0 \quad l$
 after some value, say

$$\Rightarrow l(l+1) - \lambda = 0$$

$$\Rightarrow \boxed{\lambda = l(l+1)}$$

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

$$\Theta^0(x) = 1$$

$$\Theta^1(x) = x$$

$$\Theta^2(x) = \frac{(3x^2 - 1)}{2}$$

Legendre's Polynomials.

But this was calculated for $m_e = 0$

But in general m_e may not be 0

In such a case,

$$\lambda = l(l+1)$$

and

$$|m| \leq l$$

Legendre's Polynomial $P_l(x)$ are polynomials of degree ' l '.

Associated Legendre's Polynomials are m^{th} derivatives of Legendre's Polynomial

$$m = 0, \pm 1, \pm 2, \dots \stackrel{\pm l}{\dots}$$

\Rightarrow if $|m| > l$
solution = 0

Now,

$$\Theta(x) = B \underbrace{P_l(x)}_{\text{Associated Legendre's Polynomial}} \Rightarrow \boxed{|m| \leq l}$$

Associated Legendre's Polynomials

$$= B \left[\underbrace{\frac{d^{|m|}}{dx^{|m|}}}_{\text{Legendre's Polynomial}} P_l(x) \right] (1-x^2)^{\frac{|m|}{2}}$$

I am not interested in precise value. I just want to know that there are $|m|$ derivatives.

Legendre's Polynomial

$$\text{Hence, } L^2 Y(\theta, \phi) = l(l+1) \hbar^2 Y(\theta, \phi); \quad l=0, 1, 2, \dots$$

$$\Rightarrow \underline{\text{Eigen Values}} \quad L^2 = l(l+1) \hbar^2$$

$$\Rightarrow L = 0, \sqrt{2} \hbar, \sqrt{6} \hbar, \sqrt{12} \hbar$$

Eigen Function

$$Y(\theta, \phi) = B P_l^{|m|}(\cos \theta) e^{im\phi}$$

$$P_l^{|m|}(x) = P_l^{|m|}(\cos \theta) \quad \text{as } x = \cos \theta \quad m_e = 0, \pm 1, \pm 2, \dots \pm l$$

Writing the solutions for 1st 3 states :

s state

$$l=0 \quad m_l=0 \quad \} \text{ no significance}$$

$$L^2 = 0 \quad L_z = 0$$

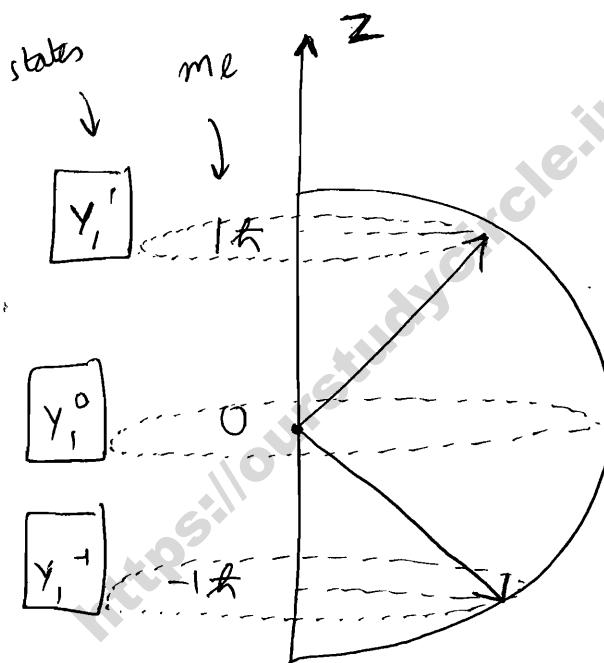
pth state

$$l=1 \quad L = \sqrt{2} \hbar$$

$$m_l = 0, 1, -1 \quad : 3 \text{ possible states } b_x, b_y, b_z$$

$$L_z = 1\hbar, -1\hbar, 0$$

Space Quantization
of Angular Momentum



$$L = R = \sqrt{2} \hbar \text{ (say)}$$

also called
 p^{th} substate

Hence Angular
Momentum Vector
can take only
discrete orientation

$$\psi(\theta, \phi) = P_l^{m_l} \cos \theta e^{im_l \phi}$$

$$P_l^{m_l} \cos \theta = \frac{d^{|m_l|}}{dx^{|m_l|}} (x^2 - 1)^{|m_l|} = \begin{cases} (x^2 - 1), & m_l = 0 \\ (2x), & m_l = \pm 1 \end{cases}$$

$$\begin{aligned} Y_1^0 &= \cos \theta e^{i(0)} = \cos \theta \\ Y_1^1 &= \cos \theta e^{i\phi} \\ Y_1^{-1} &= \cos \theta e^{-i\phi} \end{aligned}$$

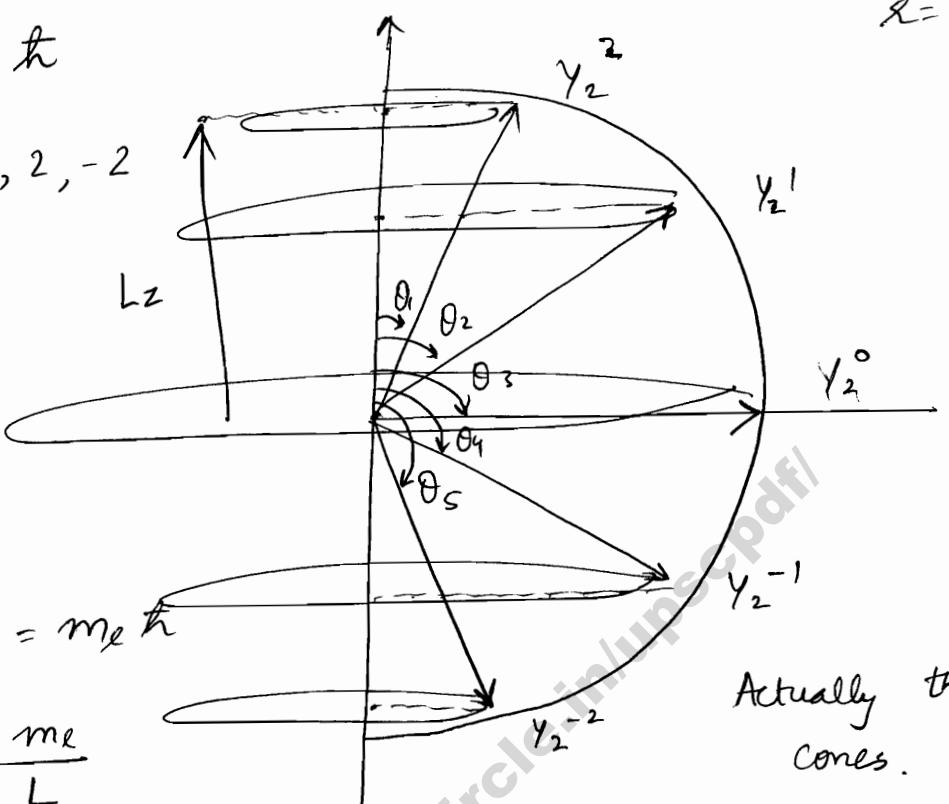
(d state) $l=2$ $d_{xy}, d_{yz}, d_{zx}, d_{x^2-y^2}, d_{z^2}$

$$L^2 = 6 \hbar^2$$

$$L = \sqrt{6} \hbar$$

$$m_e = 0, 1, -1, 2, -2$$

$$r = L = \sqrt{6} \hbar$$



$$L_z = L \cos \theta = m_e \hbar$$

$$\cos \theta = \frac{\hbar m_e}{L}$$

Actually they are cones.

$$\theta_1 = \cos^{-1} \left(\frac{2}{\sqrt{6}} \right)$$

$$\theta_2 = \cos^{-1} \left(\frac{1}{\sqrt{6}} \right)$$

$$\theta_3 = \cos^{-1} 0 = \frac{\pi}{2}$$

$$\theta_4 = \cos^{-1} \left(-\frac{1}{\sqrt{6}} \right)$$

$$\theta_5 = \cos^{-1} \left(-\frac{2}{\sqrt{6}} \right)$$

5 discrete orientations

✓ For any l quantum number state, $(2l+1)$ degenerate states.

$$T = \frac{L^2}{2I}$$

$$= \frac{l(l+1) \hbar^2}{2I}$$

Quantum Physics (10)

16/02/2023

In the last class, we have done Angular Momentum Problem

$$L^2 \Psi(\theta, \phi) = l(l+1) \hbar^2 \Psi(\theta, \phi)$$
$$l = 0, 1, 2, \dots$$

$$L_z \Psi(\theta, \phi) = m_e \hbar \Psi(\theta, \phi)$$
$$m_e = 0, \pm 1, \pm 2, \dots, \pm l$$

For a particular l , we will have $(2l+1)$ values of m_e , hence $(2l+1)$ states for given l .

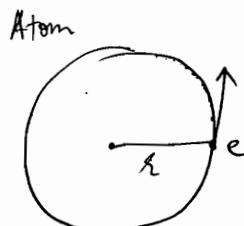
Magnitude Quantization $\Rightarrow L^2 = l(l+1)\hbar^2$ \Rightarrow along a particular direction, L can take only specific values.

Space Quantization $\Rightarrow L_z = m_e \hbar$

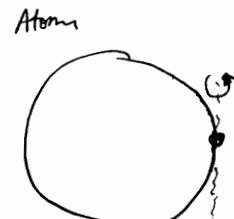
* ∞ -fold degeneracy as I can associate $f(r)$ to $\Psi(r, \theta, \phi)$ as $\Psi = f(r) Y_l^m(\theta, \phi)$ (any)

$$Y_l^{m_e}(\theta, \phi) = B P_l^{m_e}(\cos\theta) e^{im_e\phi}$$

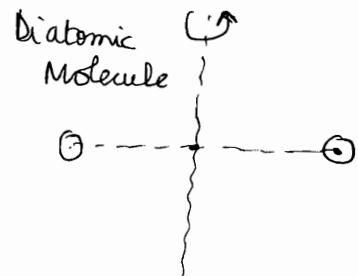
Angular Momentum is not only quantized in magnitude but also quantized in space !!



L due to orbital motion

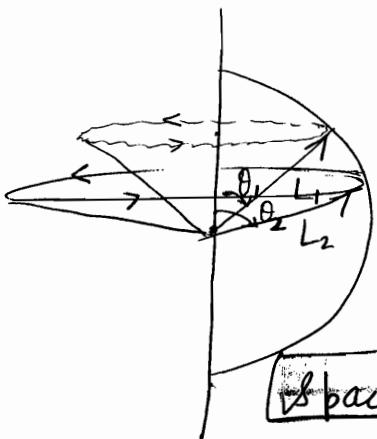


L due to spin motion



① Angular Momentum is also quantized in Nucleus.

Precession : Rotation of Angular Momentum



Note that it is example of Precession.

Space Quantization of Angular Momentum

| <u>orbital</u> | s | p | d | f | g |
|----------------|---|---|---|---|---|
| <u>l</u> | 0 | 1 | 2 | 3 | 4 |

$$\underline{L^2} \quad 0 \quad 2\hbar^2 \quad 6\hbar^2 \quad 12\hbar^2 \quad 20\hbar^2$$

in 'd' orbital

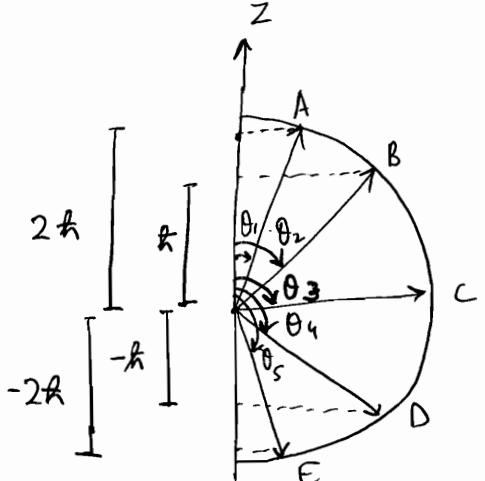
$$l=2$$

$$L^2 = 6\hbar^2 \Rightarrow L = \sqrt{6}\hbar$$

$$\text{No. of orientations} = (2l+1) = 5$$

$$= m_e \hbar$$

$$= 0, \pm 1\hbar, \pm 2\hbar$$



$$A : L_z = 2\hbar = L \cos \theta_1 \Rightarrow \theta_1 = \cos^{-1}\left(\frac{2}{\sqrt{6}}\right)$$

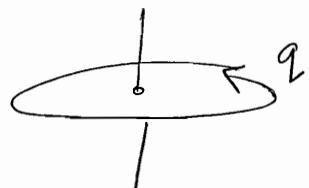
$$B : L_z = \hbar = L \cos \theta_2 \Rightarrow \theta_2 = \cos^{-1}\left(\frac{1}{\sqrt{6}}\right)$$

$$C : L_z = 0 = L \cos \theta_3 \Rightarrow \theta_3 = 90^\circ$$

$$D : L_z = -\hbar = L \cos \theta_4 \Rightarrow \theta_4 = \cos^{-1}\left(-\frac{1}{\sqrt{6}}\right)$$

$$E : L_z = -2\hbar = L \cos \theta_5 \Rightarrow \theta_5 = \cos^{-1}\left(-\frac{2}{\sqrt{6}}\right)$$

Angular Momentum, broadly means, rotation about some axis. When charged particle rotates, it is equivalent to current carrying loop.



$$I = \left(\frac{q}{T} \right) = qV = \frac{q\omega}{2\pi}$$

Electron, Proton, Neutron are $\frac{1}{2}$ spin particles.

Every current carrying loop is equivalent to a magnetic dipole.

$$B = \frac{\mu_0 I}{2r}; \quad \boxed{\vec{\mu} = \vec{IA}} = \frac{q\omega}{2\pi} \pi r^2$$

dipole moment
~~~~~

$$= \left( \frac{q\omega r^2}{2} \right)$$

If +vely charged particle,  $\mu$  and  $L$  are in same direction.

$$= \frac{mq\omega r^2}{2m}$$

$$= \left( \frac{q}{2m} \right) \vec{L}$$

If -vely charged particle,  $\mu$  and  $L$  are opposite.

If a charge particle has angular momentum  $\Rightarrow$  it has a dipole moment.

Now every atom has rotating charged particles,  
 $\Rightarrow$  it has intrinsic magnetic field.

Hence this is the reason of observed rotation of  $\vec{L}$  !!

$$\vec{T} = \vec{\mu} \times \vec{B}$$

Torque tries to rotate  $\vec{\mu}$  in direction of field.

$\Rightarrow$  Torque will rotate  $\vec{L}$ ; hence precession of Angular Momentum

$$\vec{L} = \vec{\mu} \times \vec{B}$$

$$\frac{d\vec{L}}{dt} = \frac{q}{2m} \vec{L} \times \vec{B}$$

: Precession  
Motion

Prerequisite of Precession is Angular Momentum  $\vec{L}$ .  
Hence no precession in 's' orbital, as  $L_s = 0$

$$\vec{\mu} = \frac{q}{2m} \vec{L}$$

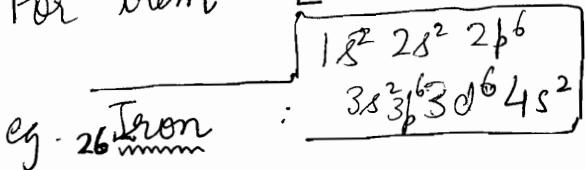
$$\frac{\text{Magnetic Moment}}{\text{Angular Momentum}} = \frac{\mu}{L} = \left( \frac{q}{2m} \right) = \text{const}$$

"GYRO MAGNETIC RATIO"

Note that for 's' orbital for which  $L=0$ , gyromagnetic ratio is 2 times  $\left( \frac{q}{2m} \right)$  i.e.  $\left( \frac{q}{m} \right)$

It is valid for ferromagnetic materials.

For them  $L=0$



For them

$$\frac{\text{Spin Magnetic Moment}}{\text{Spin Angular Momentum}} = \left( \frac{q}{m} \right)$$

Hence, classically we were not able to explain gyromagnetic ratio. We need quantum mechanical concept of spin to explain this.

$$[S^2 = s(s+1) \hbar^2]$$

## Spin Angular Momentum

$$S_z = m_s \hbar$$

$$m_s : -s \text{ to } +s$$

$$= \left( \frac{-1}{2}, \frac{1}{2} \right) \text{ for electron}$$

Why spin to be introduced?

- 1) To explain Gyromagnetic ratio of Ferromagnetic materials ( $l=0$ )

$$= |\mu_s| = \left( \frac{e}{m} \right)$$

→ These are called 'Pre Spin' Riddles

- 2) Fine structure of spectral lines

- 3) Zeeman Effect

- 4) Stern - Gerlach Experiment [This experiment fixes  $\mu_s = \left( \frac{1}{2} \right)$  for electron]

- 5) Also apart from  $0, 2\hbar^2, 6\hbar^2, 12\hbar^2 \dots$ , we have also observed values of angular momentum like

$$\frac{3}{4}\hbar^2, \frac{15}{4}\hbar^2 \dots$$

$$(s=\frac{1}{2}) \quad (s=\frac{3}{2})$$

Hence spin required to explain this.

① Since 's' values are quantized, it is not a simple classical motion but rather a quantum mechanical concept.

Goud Schmidt and Uhlenbeck proposed in 1925 the idea of spin for particles.

[ 15p at Postcard at 300<sup>2</sup> ₹ 5/- ]

## Properties of Angular Momentum

$$\begin{aligned} \vec{L} \times \vec{L} &= i\hbar \vec{L} \\ \vec{S} \times \vec{S} &= i\hbar \vec{S} \\ \vec{J} \times \vec{J} &= i\hbar \vec{J} \\ \vec{I} \times \vec{I} &= i\hbar \vec{I} \end{aligned}$$

★ Note that these are operators and not numbers  
 $AB \neq BA$   
Hence  $\vec{L} \times \vec{L} \neq 0$

In this cross product, we have 3 results :

$$\begin{aligned} [L_x, L_y] &= i\hbar L_z \\ [L_y, L_z] &= i\hbar L_x \\ [L_z, L_x] &= i\hbar L_y \end{aligned}$$

Note that the 3 are cyclic results

Commutation Result satisfied by Angular Momentum Operators.

Cross Product Expansion if 2<sup>nd</sup> row variable is multiplied to 3<sup>rd</sup> row variable and never vice versa.

$$\begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ L_x & L_y & L_z \\ L_x & L_y & L_z \end{vmatrix}$$

$$\Rightarrow \hat{i} [ L_y L_z - L_z L_y ] +$$

$$\hat{j} [ L_z L_x - L_x L_z ] +$$

$$\hat{k} [ L_x L_y - L_y L_x ]$$

$$= i\hbar [ L_x \hat{i} + L_y \hat{j} + L_z \hat{k} ]$$

NOTE FOR 1<sup>st</sup> TIME IN LIFE .... 2<sup>nd</sup> TERM OF CROSS PRODUCT IS NOT NEGATIVE OR OPPOSITE.... ITS SIMPLY THE NEXT TWO ROWS 3<sup>rd</sup> and 1<sup>st</sup> are PLACED OPPOSITE  
NOTE THAT CYCLIC ORDER IS FOLLOWED

$$\begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \end{vmatrix} = i(a_2 b_3 - a_3 b_2) + j(a_3 b_1 - a_1 b_3) + k(a_1 b_2 - a_2 b_1)$$

$$\Rightarrow L_y L_z - L_z L_y = i\hbar L_x$$

$$L_z L_x - L_x L_z = i\hbar L_y$$

$$L_x L_y - L_y L_x = i\hbar L_z$$

$\checkmark$  if  $[A B] = 0 \Rightarrow$  they can be measured in same state.  
 $\Rightarrow$  they can be measured simultaneously with similar levels of accuracy.

We need to prove any 1 of them ; similarly other 2 can be proved.

Now we know

$$L_x = Y P_z - Z P_y = -i\hbar \left[ y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right]$$

$$L_y = Z P_x - X P_z = -i\hbar \left[ z \frac{\partial}{\partial x} - x \frac{\partial}{\partial z} \right]$$

$$L_z = X P_y - Y P_x = -i\hbar \left[ x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right]$$

To prove  $[L_x L_y] = i\hbar L_z$

$\checkmark$  No need to open into derivatives  
just use  $[AB, C]$  and  $[A, BC]$  properties repeatedly along with  $[x p_x] = i\hbar$

$$\text{L.H.S.} = L_x L_y - L_y L_x$$

$$L_x L_y = -\hbar^2 \left[ y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right] \left[ z \frac{\partial}{\partial x} - x \frac{\partial}{\partial z} \right]$$

$$L_y L_x = +\hbar^2 \left( z \frac{\partial}{\partial x} - x \frac{\partial}{\partial z} \right) \left( y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right)$$

$$L_x L_y = -\hbar^2 \left( y \frac{\partial}{\partial z} \left( z \frac{\partial}{\partial x} \right) - y \frac{\partial}{\partial z} \left( x \frac{\partial}{\partial z} \right) - z \frac{\partial}{\partial y} \left( z \frac{\partial}{\partial x} \right) + z \frac{\partial}{\partial y} \left( x \frac{\partial}{\partial z} \right) \right)$$

$$= -\hbar^2 \left[ y \frac{\partial^2}{\partial x \partial z} + y \cancel{z \frac{\partial^2}{\partial z \partial x}} - \cancel{x y \frac{\partial^2}{\partial z \partial y}} - \cancel{z^2 \frac{\partial^2}{\partial x \partial y}} + \cancel{x z \frac{\partial^2}{\partial y \partial z}} \right]$$

$$L_y L_x = -\hbar^2 \left[ z \frac{\partial}{\partial x} \left( y \frac{\partial}{\partial z} \right) - z \frac{\partial}{\partial x} \left( z \frac{\partial}{\partial y} \right) - x \frac{\partial}{\partial z} \left( y \frac{\partial}{\partial z} \right) + x \frac{\partial}{\partial z} \left( z \frac{\partial}{\partial y} \right) \right]$$

$$= -\hbar^2 \left[ \cancel{zy \frac{\partial^2}{\partial x \partial z}} - \cancel{z^2 \frac{\partial^2}{\partial x \partial y}} - \cancel{x y \frac{\partial^2}{\partial z \partial z}} + x \frac{\partial}{\partial y} + \cancel{x z \frac{\partial^2}{\partial z \partial y}} \right]$$

Subtracting,

$$[L_x \ L_y] = -\hbar^2 \left[ y \frac{\partial}{\partial x} - x \frac{\partial}{\partial y} \right]$$

$$= \cancel{i\hbar^2(-L_2)}$$

fit

$$= i\hbar L_z$$

~~~~~

$$= \underline{\underline{\text{R.H.S}}}$$

Hence Proved.

Similar relation: $[S_x \ S_y] = i\hbar S_z$

In Matrix $[A \ B, C] = A[B, C] + [A, C]B$

~~(2)~~ $[L^2 \ L_x] = 0$

$$[L^2 \ L_y] = 0$$

$$[L^2 \ L_z] = 0$$

We can prove any 1.

$$L^2 - L_z^2 = \underbrace{L_x^2 + L_y^2}_{\text{error in measurement}}$$

1 component can be measured along with $|L\rangle$ physical interpretation
with same accuracy.

Error will be there in other 2 components.

$$A^2 A = AA^2 = A^3 \quad (\text{in matrix})$$

$$[L^2, L_z] = 0 \quad (\text{To prove})$$

LHS

$$= [L_x^2 + L_y^2 + L_z^2, L_z]$$

$$= [L_x^2, L_z] + [L_y^2, L_z] + 0$$

Since operator can be written in matrix form, applying an operator is equivalent to Matrix Multiplication....

Matrix Multiplication is associative...

$$= L_x [L_x L_z] + [L_x L_z] L_x$$

$$+ L_y [L_y L_z] + [L_y L_z] L_y$$

$$= L_x (-i\hbar L_y) + L_y i\hbar L_x - i\hbar L_y L_x$$

$$+ L_y i\hbar L_x + i\hbar L_x L_y$$

$$= 0$$

$$= \underline{\underline{R.H.S.}}$$

We can write:

$$\boxed{[L^2, L_z] | l, m \rangle = 0}$$

$\psi_{l,m}$: state representation
of
Angular Momentum

$$[x, p_x] |\psi\rangle$$

$$= \cancel{\cdot} \cdot x - i\hbar \frac{\partial}{\partial x} \psi + i\hbar \frac{\partial}{\partial x} (x\psi)$$

$$= -ix\hbar \cancel{\left(\frac{\partial \psi}{\partial x} \right)} + i\hbar \psi + i\hbar x \cancel{\left(\frac{\partial \psi}{\partial x} \right)}$$

$$= i\hbar |\psi\rangle$$

$$\Rightarrow [x \ p_x] |\psi\rangle = i\hbar |\psi\rangle$$

Hence, it means x, p_x cannot be simultaneously measured with similar level of accuracy.

$$[x^2, p_x] |\psi\rangle = 2i\hbar x |\psi\rangle$$

$$[x^n, p_x] |\psi\rangle = n i\hbar x^{n-1} |\psi\rangle \quad \checkmark \text{ Perfect}$$

1 line
proof

Similarly

$$[x, p_x^m] |\psi\rangle = m i\hbar p_x^{m-1} |\psi\rangle \quad \checkmark \text{ Perfect} \quad \text{Proof by induction}$$

$$[L_x, x] \psi = ? = \text{say, } \lambda \psi$$

$$\begin{aligned} & L_x x \psi - x L_x \psi \\ &= -i\hbar \left[\left(y \frac{\partial}{\partial x} - z \frac{\partial}{\partial y} \right) (x \psi) \right] + x i\hbar \left[y \frac{\partial}{\partial x} \psi - z \frac{\partial}{\partial y} \psi \right] \\ &= \underline{0} \end{aligned}$$

$$[L_x, \chi] = 0$$

← can be measured simultaneously

$$[L_x, y] \neq 0$$

← cannot be measured simultaneously

$$[L_x, y] = i\hbar z$$

- ★ Remember that all degenerate states m_i 's of a quantum number 'l' are assumed to be orthonormal for all of our analysis.
- ★ If non-degenerate eigenvalue of L_z (or L^2) , only then it commute with L^2 (or L_z) otherwise not necessary but we can surely find n commuting eigenfunctions for a n-level degeneracy.

Quantum Physics (1)

17/02/12

Ladder Operations

$$L_+ = L_x + iL_y$$

$$L_- = L_x - iL_y$$

$\star L_{(+)}$ and $L_{(-)}$ are not Hermitian operators but adjoints of each other
 i.e. $\langle L_{(+)} \psi_1 | \psi_2 \rangle = \langle \psi_1 | L_{(-)} \psi_2 \rangle$
 & $\langle L_{(-)} \psi_1 | \psi_2 \rangle = \langle \psi_1 | L_{(+)} \psi_2 \rangle$

$$[L^2, L_+] = 0 = [L^2, L_-] \quad \text{--- (1)}$$

↗ used to show some

L_{\pm} : ladder Operators

3 Properties of adjoints

$$\begin{aligned} ① (A^{ad})^{ad} &= A \\ ② (AB)^{ad} &= B^{ad} A^{ad} \\ ③ (A+B)^{ad} &= A^{ad} + B^{ad} \end{aligned}$$

$$[L^2, L_+] = [L^2 L_x] + i [L^2 L_y] = 0 + 0 = 0$$

$$[L^2, L_{(-)}] = [L^2 L_x] - i [L^2 L_y] = 0 - 0 = 0$$

O Bra $\langle \psi_1 |$:- symbol to indicate the 1st function in a scalar product of state $|\psi_1\rangle$ with $|\psi_2\rangle$.

$$\langle \psi_1 | \psi_2 \rangle = \int_{\text{space}} \psi_1^* \psi_2 \, dx$$

The scalar product is NON COMMUTATIVE.

$$[L_+, L_z]$$

$$= [L_x + iL_y, L_z]$$

$$= [L_x L_z] + i [L_y L_z] \\ = -i\hbar L_y + i\hbar L_x$$

$$= \hbar L_+$$

④ If $|\psi\rangle = c_1 [i|\alpha\rangle + 2|\beta\rangle]$

where $|\alpha\rangle$ and $|\beta\rangle$ are orthonormal wave functions

$$\Rightarrow \langle \psi | = c_1 [-i \langle \alpha | + 2 \langle \beta |] = (\langle \psi |)^*$$

$$\text{and} \\ |\phi\rangle = c_2 [|\alpha\rangle - i|\beta\rangle]$$

i.e.

↗ used to
mt or
m-1

$$[L_z, L_+] = \hbar L_+$$

$$\Rightarrow \langle \psi | \phi \rangle$$

$$= \langle \psi | * | \phi \rangle$$

$$= c_1 [-i \langle \alpha | + 2 \langle \beta |] * [c_2 (|\alpha\rangle - i|\beta\rangle)]$$

$$= c_1 c_2 [-i \langle \alpha | \alpha \rangle - 2i \langle \beta | \alpha \rangle]$$

$$= -3i c_1 c_2$$

Similarly,

$$[L_z, L_-] = -\hbar L_-$$

Also, since $L_+ = L_x + iL_y$
and $L_- = L_x - iL_y$

$$\left\{ \begin{array}{l} \langle L_{(+)} |\psi_1\rangle = \langle \psi_1 | L_{(+)} \rangle \\ \langle L_{(-)} |\psi_1\rangle = \langle \psi_1 | L_{(-)} \rangle \end{array} \right.$$

★ $\langle \psi_1 | A | \psi_2 \rangle$ normally means
 $\langle \psi_1 | (A \psi_2) \rangle = \int_{\text{space}} \psi_1^* (A \psi_2) dx$
 For Hermitian operators only,
 $\langle \psi_1 | A \psi_2 \rangle = \langle A \psi_1 | \psi_2 \rangle$
 $= \int_{\text{space}} (A \psi_1)^* \psi_2 dx$

i.e. For Hermitian A can be associated with bra or ket.

Now we have shown,

$$[L_z, L_+] = L_z L_{(+)} - L_{(+)} L_z = \hbar L_+$$

Operating it on a wave function

$$\Rightarrow [L_z, L_+] |l, m\rangle = \hbar L_+ |l, m\rangle$$

$$\Rightarrow L_z L_{(+)} |l, m\rangle - L_{(+)} \underbrace{L_z}_{|l, m\rangle} = \hbar L_{(+)} |l, m\rangle = \hbar (l+1) |l+1, m\rangle$$

$$\Rightarrow L_z L_+ |l, m\rangle - L_{(+)} m \hbar |l, m\rangle = \hbar L_{(+)} |l, m\rangle$$

$$\Rightarrow L_z \underbrace{[L_{(+)} |l, m\rangle]}_{|l, m\rangle} = \hbar (m+1) \underbrace{[L_+ |l, m\rangle]}_{|l, m\rangle}$$

Also from ①
 $L^2 [L_{(+)} |l, m\rangle] = L_+ [L^2 |l, m\rangle] = L_+ [l(l+1) \hbar^2 |l, m\rangle]$

This shows
 that $[L_{(+)} |l, m\rangle]$
 is an eigen state
 of L^2 with eigen value
 $l(l+1) \hbar^2$

∴ Hence $[L_+ |l, m\rangle]$ is eigen state of L_z with eigen value of $(m+1)\hbar$. But for operator, eigen state corresponding to eigen value $(m+1)\hbar$ is $|l, m+1\rangle$.

Hence job of $L_{(+)}$ operator is to raise the

state of eigenfunction
 for which eigenvalue is raised by 1.

Similarly job of L_- operator is to drop the eigen value by 1 to lower level.

$$L_z [L_{(-)} |l, m\rangle] = \hbar (m-1) [L_{(-)} |l, m\rangle]$$

$$\text{Also, } [L^2, L_z] |L_+ |l, m\rangle = 0$$

★ From these two, it means $L_{(+)}$ raises $|l, m\rangle$ to $|l, m+1\rangle$

Note that now

since states as changes, it is not eigenvalue problem

i.e. let C_1, C_2 be constant associated with $L_{(+)}$ & $L_{(-)}$ operators respectively.

$$\begin{aligned} L_{(+)} |l, m\rangle &= C_1 |l, m+1\rangle \\ L_{(-)} |l, m\rangle &= C_2 |l, m-1\rangle \end{aligned}$$

$$\begin{aligned} \downarrow \\ L_{(+)} |l, m\rangle &= C_1 |l, m+1\rangle \end{aligned}$$

$$\Rightarrow \langle L_{(+)} | l, m \rangle \langle L_{(+)} | l, m \rangle = |C_1|^2 - \textcircled{1} \quad \left. \begin{array}{l} \text{because} \\ |l, m\rangle \& |l, m+1\rangle \\ \text{are orthonormal} \\ \text{vectors!!} \end{array} \right\}$$

$$\langle L_{(-)} | l, m \rangle \langle L_{(-)} | l, m \rangle = |C_2|^2 - \textcircled{2}$$

From ①, $\langle l, m | L_{(+)} L_{(+)} | l, m \rangle = |C_1|^2 - \textcircled{3}$

using the property of Hermitian adjoints

Similarly

From ②

$L_{(+)} \& L_{(-)}$ are adjoints

$$\langle l, m | L_{(+)} L_{(-)} | l, m \rangle = |C_2|^2 - \textcircled{4}$$

From ③ & ④

$$\Rightarrow \left\{ \begin{array}{l} |C_1|^2 \Leftrightarrow \text{expectation value of } L_{(-)} L_{(+)} \\ |C_2|^2 \Leftrightarrow \text{expectation value of } L_{(+)} L_{(-)} \end{array} \right\} \text{actually in these 2 RHS has no real meaning!!}$$

Now we can write,

$$L_- L_+ = (L_x - iL_y) (L_x + iL_y)$$

$$= L_x^2 + i(L_x L_y - L_y L_x) + L_y^2$$

$$= L^2 - L_z^2 + i [L_x L_y]$$

$$= L^2 - L_z^2 + i \hbar L_z$$

$$= L^2 - L_z^2 - \hbar L_z \quad \begin{array}{l} \star \langle l, m | L_z^2 | l, m \rangle \\ \Leftrightarrow \langle \psi(l, m) | L_z^2 \psi(l, m) \rangle \\ \Leftrightarrow \langle \psi(l, m) | L_z L_z \psi(l, m) \rangle \end{array}$$

$$\Leftrightarrow \langle \psi(l, m) | L_z \cancel{m \neq \psi(l, m)} \rangle$$

$$\Leftrightarrow (m\hbar) \langle \psi(l, m) | L_z \psi(l, m) \rangle$$

$$\Leftrightarrow (m\hbar)^2 \langle \psi(l, m) | \psi(l, m) \rangle = (m\hbar)^2$$

Putting it in ③,

$$\langle l, m | L^2 - L_z^2 - \hbar L_z | l, m \rangle = |C_1|^2$$

$$|C_1|^2 = \langle l, m | L^2 | l, m \rangle - \underbrace{\langle l, m | L_z^2 | l, m \rangle}_{m^2 \hbar^2} - \hbar \langle l, m | L_z | l, m \rangle$$

$$= l(l+1)\hbar^2 - m^2\hbar^2 - m\hbar^2$$

$$\Rightarrow |C_1|^2 = [l(l+1) - m(m+1)] \hbar^2$$

$$\Rightarrow |C_1|^2 = [(l^2 - m^2) + (l-m)] \hbar^2$$

$$|C_1|^2 = [(l-m)(l+m+1)] \hbar^2$$

We are given $Y_3^0 \leftarrow^m l$

We can calculate, Y_3^{-1} , Y_3^{-1} , Y_3^2 , Y_3^{-2} , ...

$$\checkmark L_{(+)} |l, m\rangle = \sqrt{(l-m)(l+m+1)} \hbar |l, m+1\rangle$$

$$\checkmark L_{(-)} |l, m\rangle = \sqrt{(l+m)(l-m+1)} \hbar |l, m-1\rangle$$



If I require, L_x or L_y anywhere From these 2 its clear that $L_{(+)} |2, 2\rangle = 0$

$$L_{(+)} = L_x + iL_y$$

$$L_{(-)} |2, -2\rangle = 0$$

$$L_{(-)} = L_x - iL_y$$

$$\Rightarrow L_x = \frac{L_{(+)} + L_{(-)}}{2} \quad ;$$

$$L_y = \frac{L_{(+)} - L_{(-)}}{2i}$$

$$\text{If I require } \Delta L_x = \sqrt{\langle L_x^2 \rangle - \langle L_x \rangle^2}$$

$$L_x^2 = \frac{(L_{(+)} + L_{(-)})(L_{(+)} + L_{(-)})}{2 \cdot 2}$$

$$= \frac{1}{4} \left[L_{(+)}^2 + L_{(-)}^2 + L_{(+)} L_{(-)} + L_{(-)} L_{(+)} \right]$$

Let us analyze this via a problem,

$$\text{Q1} \quad Y_2^1 = \frac{1}{\sqrt{15}} \cos^2 \theta e^{i\phi} \quad (\text{given})$$

find ΔL_x .

We are given $l=2$ ✓
 $m=1$ ✓

$$\Rightarrow Y_2^1 = |2,1\rangle$$

$$\langle L_x \rangle = \langle 2,1 | \frac{L_{(+)} + L_{(-)}}{2} | 2,1 \rangle$$

$$= \frac{1}{2} \langle 2,1 | L_{(+)} | 2,1 \rangle + \frac{1}{2} \langle 2,1 | L_{(-)} | 2,1 \rangle$$

$$L_{(+)} |2,1\rangle = \sqrt{(2-1)(2+1+1)} \hbar |2,2\rangle$$

Now $|2,1\rangle$ and $|2,2\rangle$ are orthogonal
 Hence upon multiplying, it gives 0.

$$\Rightarrow \langle L_x \rangle = 0$$

$$\langle L_x^2 \rangle = \frac{1}{4} \langle 2,1 | L_{(+)}^2 + L_{(-)}^2 + L_+ L_- + L_- L_+ | 2,1 \rangle$$

↑ ↑

it will give 0

$$\Rightarrow \langle L_x^2 \rangle = \frac{1}{4} \langle 2,1 | L_{(+)} L_{(-)} + L_{(-)} L_{(+)} | 2,1 \rangle + \frac{1}{4} \langle 2,1 | L_{(-)} L_{(+)} | 2,1 \rangle$$

\Rightarrow first applying $L_{(-)}$, we get from 1st term

$$\frac{1}{4} \langle 2,1 | L + \sqrt{6}\hbar | 2,0 \rangle \quad [\text{do not forget } \sqrt{ }]$$

$$= \frac{\sqrt{6}\hbar}{4} \langle 2,1 | L + 12,0 \rangle \quad [\text{do not forget } \hbar]$$

$$= \frac{\sqrt{6}}{4} \langle 2,1 | \sqrt{6}\hbar | 2,1 \rangle \quad \text{Similarly,}$$

$$= \frac{6\hbar^2}{4} \langle 2,1 | 12,1 \rangle$$

$$= \left(\frac{6\hbar^2}{4} \right)$$

Hence, just with knowledge of Quantum Numbers (m, l) we have calculated $\langle L_x \rangle, \langle L_x^2 \rangle$

Coming to Orbitals, $\langle L_y \rangle, \langle L_y^2 \rangle$

$$\frac{1}{4} \langle 2,1 | L_{(-)} L_{(+)} | 2,1 \rangle$$

$$= \frac{1}{4} \langle 2,1 | L_{(-)} 2\hbar | 2,2 \rangle$$

$$= \frac{1}{4} \cdot 2\hbar \langle 2,1 | 2\hbar | 2,1 \rangle$$

$$\hbar^2 \Rightarrow \langle L_z^2 \rangle = \frac{5}{2} \hbar^2$$

$$\Delta L_x = \sqrt{\frac{5}{2}} \hbar$$

Similar to Orbital Angular Momentum, we have Spin Angular Momentum

$$S^2 |s, m\rangle = s(s+1) \hbar^2 |s, m\rangle$$

$$S_z |s, m\rangle = m_s \hbar |s, m\rangle$$

Note that 's' and 'm' are pure numbers as \hbar^2 and \hbar have already been separated !!

$$s = \left(\frac{1}{2} \right)$$

$$m_s = -s \text{ to } +s \quad [-s, -s+1, \dots, s-1, s] \quad (2s+1 \text{ values})$$

$$\left. \begin{aligned} S_z |s, m\rangle &= \pm \frac{1}{2} \hbar |s, m\rangle \\ S_y |s, m\rangle &= \pm \frac{1}{2} \hbar |s, m\rangle \\ S_x |s, m\rangle &= \pm \frac{1}{2} \hbar |s, m\rangle \end{aligned} \right\} \quad \begin{array}{l} \text{can be in} \\ \text{any direction} \end{array}$$

We have all similar results,

$$S_{(+)} = [S_x + iS_y]$$

$$S_{(-)} = [S_x - iS_y]$$

$$S_{(+)} |s, m\rangle = \sqrt{(s-m)(s+m+1)} \hbar |s, m\rangle$$

$$S_{(-)} |s, m\rangle = \sqrt{(s+m)(s-m+1)} \hbar |s, m\rangle$$

→ if $s = \frac{3}{2}\hbar$
 m has $(2s+1) = 4$ values,
 $-\frac{3\hbar}{2}, -\frac{1\hbar}{2}, \frac{1\hbar}{2}, \frac{3\hbar}{2}$

Now all operators can be represented as matrices of order n
where n eigen values are these. And corresponding n orthogonal eigen functions

⇒ for $s = \frac{1}{2}$ SPIN $\frac{1}{2}$ PROBLEM $|\psi_i\rangle_s$

there are only 2 eigen values of S_x, S_y, S_z

hence represented by 2×2 matrix.

They are called Pauli Spin Matrices (2×2)

eigen values of $S_x = \pm \frac{1}{2}\hbar$

⇒ $S_x = \frac{1}{2}\hbar \sigma_x$ EV. $(\sigma_x) = \pm 1$

operator in matrix form

σ_x is 2×2 matrix whose eigen value is ± 1

similarly,

$$S_y = \frac{1}{2}\hbar \sigma_y$$

$$\text{EV.}(\sigma_y) = \pm 1$$

$$S_z = \frac{1}{2}\hbar \sigma_z$$

$$\text{EV.}(\sigma_z) = \pm 1$$

2×2 matrices
with
eigen value is
 ± 1

$$S^2 = S_x^2 + S_y^2 + S_z^2$$

$$= \frac{3}{4}\hbar^2$$

$$= s(s+1)\hbar^2$$

$$= S^2$$

$$S_x \Psi_1 = \frac{1}{2} \hbar \Psi_1 \quad \left. \begin{array}{l} \\ \end{array} \right\} \text{Upon measurement, we can have } 2 \text{ values.}$$

$$S_x \Psi_2 = -\frac{1}{2} \hbar \Psi_2$$

i.e. $S_x \left| \frac{1}{2}, \frac{1}{2} \right\rangle = \left(\frac{1}{2} \right) \hbar \left| \frac{1}{2}, \frac{1}{2} \right\rangle$

$$S_x \left| \frac{1}{2}, -\frac{1}{2} \right\rangle = \left(-\frac{1}{2} \right) \hbar \left| \frac{1}{2}, -\frac{1}{2} \right\rangle$$

We write $\left| \frac{1}{2}, \frac{1}{2} \right\rangle$ as X_+ : spin up state \uparrow
or
spin up vector

$\left| \frac{1}{2}, -\frac{1}{2} \right\rangle$ as X_- : spin down state \downarrow
or
spin down vector

Now we can write,

| | |
|--|---|
| $S_x X_{(+)} = \frac{1}{2} \hbar X_{(+)}$ | $\leftarrow \frac{1}{2} \hbar \text{ spin Eigen Value Problem}$ |
| $S_x X_{(-)} = -\frac{1}{2} \hbar X_{(-)}$ | |

State of any $\frac{1}{2}$ spin particle

$$|X\rangle = c_1 |X_{(+)}\rangle + c_2 |X_{(-)}\rangle$$

Upon normalization

$$\langle X | X \rangle = 1 \Rightarrow c_1^2 + c_2^2 = 1$$

$$S_x \underset{(2 \times 2)}{\cancel{X_{(+)}}} = \frac{1}{2} \hbar \left[X_{(+)} \right]_{2 \times 1} \quad \leftarrow \text{Matrix Representation}$$

Hence state is a ~~vector~~ column matrix

Orthonormal vectors

$$|X\rangle = \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = c_1 \begin{bmatrix} 1 \\ 0 \end{bmatrix} + c_2 \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

* In general $\psi = c_1 \phi_1 + c_2 \phi_2 + c_3 \phi_3 \dots = c_1 \begin{bmatrix} 1 \\ 0 \end{bmatrix} + c_2 \begin{bmatrix} 0 \\ 1 \end{bmatrix} + \dots$

$|X_{(+)}\rangle = \left| \frac{1}{2}, \frac{1}{2} \right\rangle$ = Matrix Representation $\begin{bmatrix} 1 \\ 0 \end{bmatrix}$

$$|X_{(-)}\rangle = \left| \frac{1}{2}, -\frac{1}{2} \right\rangle$$
 = Matrix Representation $\begin{bmatrix} 0 \\ 1 \end{bmatrix}$

Also note, orthogonality, $\langle X_{(+)} | X_{(-)} \rangle = \boxed{0}$ $[1 \ 0] \begin{bmatrix} 0 \\ 1 \end{bmatrix} = [0]$

① Tut 3

- ① (i) only function of ϵ
no dependence on θ and ϕ
 $\Rightarrow l=0$

$$(ii) \vec{S} \times \vec{S} = i\hbar \vec{S}$$

$$[S^2, S_x] = 0$$

$$S_x S_y + S_y S_x = 0 \quad ; \quad \text{Anti Commutation}$$

or

$$\tau_x \tau_y + \tau_y \tau_x = 0$$

② $S^2 = \frac{3}{4} \hbar^2$

$$16 \quad X = A \begin{pmatrix} 3i \\ 4 \end{pmatrix}$$

$$\langle X | X \rangle = 1$$

$$\langle X | = A^* \begin{bmatrix} -3i & 4 \end{bmatrix} \quad \textcircled{*}$$

$$\langle X | X \rangle = |A|^2 \begin{bmatrix} -3i & 4 \end{bmatrix} \begin{bmatrix} 3i \\ 4 \end{bmatrix} = |A|^2 (9 + 16) = 1$$

$$\Rightarrow |A| = \underline{\frac{1}{5}}$$

$$\Rightarrow X = \frac{1}{5} \begin{bmatrix} 3i \\ 4 \end{bmatrix}$$

We require, $\langle S_x \rangle$ and $\langle S_x^2 \rangle$ i.e. $\Delta S_x = \sqrt{\langle S_x^2 \rangle - \langle S_x \rangle^2}$

We know,

$$\langle S_x \rangle = \langle X | S_x | X \rangle$$

But what is S_x ??

$$S_x = \underbrace{\frac{1}{2} \hbar \sigma_x}_{\text{matrix form}} \quad \&$$

$$S_x = \underbrace{\frac{S_{(+)} + S_{(-)}}{2}}_{\text{relation to ladder operators.}}$$

We know

$$S_x = \begin{bmatrix} \langle X_+ | S_x | X_+ \rangle \\ \langle X_- | S_x | X_+ \rangle \end{bmatrix}$$

$$\langle X_+ | S_x | X_- \rangle$$

refer
[19.5] H.C. Verma
for its
derivation P. 264

$$= \frac{1}{2} \begin{bmatrix} \langle X_+ | S_{(+)} + S_{(-)} | X_+ \rangle & \dots \\ \dots & \dots \end{bmatrix}$$

or
refer to end of
this lecture !!

$$\langle X_+ | S_+ | X_+ \rangle + \langle X_+ | S_- | X_- \rangle$$

$$\text{Note that } S_{(+)} X_+ = 0 \quad S_{(-)} X_+ = 0$$

$$S_{(+)} X_- = \sqrt{\left(\frac{1}{2} + \left(\frac{1}{2}\right)\right) \left(\frac{1}{2} - \frac{1}{2} + 1\right)} \hbar = \hbar X_{(+)}$$

i.e.

$$S_{(+)} X_{(-)} = \hbar X_{(+)} \quad \boxed{S_{(+)} X_{(-)} = \hbar X_{(+)}}$$

$$S_{(-)} X_{(+)} = \hbar X_{(-)} \quad \boxed{S_{(-)} X_{(+)} = \hbar X_{(-)}}$$

$$S_{(+)} X_{(+)} = 0$$

$$S_{(-)} X_{(-)} = 0$$

$$\Rightarrow S_x = \frac{1}{2} \begin{bmatrix} 0 & \hbar \\ \hbar & 0 \end{bmatrix} = \frac{1}{2}\hbar \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \underbrace{\qquad}_{[\sigma_x]}$$

$$\boxed{\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}}$$

$$\text{Now } S_y = \frac{1}{2i} \left[\langle x_+ | S_{(+)} - S_{(-)} | x_- \rangle \dots \right]$$

$$= \frac{1}{2i} \begin{bmatrix} 0 & \hbar \\ -\hbar & 0 \end{bmatrix}$$

$$= \frac{1}{2} \hbar \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix} \underbrace{\qquad}_{[\sigma_y]}$$

$$\boxed{\sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}}$$

L_x and L_y knowledge from of $L_{(+)}$ and $L_{(-)}$ while L_z from commutation of $[L_x, L_y]$

We know L_x, L_y ; L_z can be calculated easily by Commutation Results.

$$\text{i.e. } S_z = S_x S_y - S_y S_x$$

$$\underline{s_x s_y - s_y s_x = i\hbar s_z} \quad - \textcircled{1}$$

$$\Rightarrow s_z = \frac{1}{2} \hbar \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$\sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

To prove

$$\underline{s_x s_y + s_y s_x = 0} \quad - \textcircled{2}$$

$$\frac{1}{i\hbar} [i\hbar s_x s_y + i\hbar s_y s_x] \quad [\text{multiply \& divide by } i\hbar]$$

$$= \frac{1}{i\hbar} [s_x [s_z, s_x] + [s_z, s_x] s_x]$$

$$= \frac{1}{i\hbar} [s_x s_z s_x - s_x^2 s_z + s_z s_x^2 - \cancel{s_x s_z s_x}]$$

$$= 0 \quad \cancel{\frac{s_x^2 = I}{s_y^2 = I}} = \underbrace{[1 \ 0][0 \ 1][1 \ 0]}_{[0 \ 1][0 \ 1]} - \underbrace{[0 \ 1][0 \ 1][1 \ 0]}_{[1 \ 0][1 \ 0]}$$

$$= [0 \ 1][0 \ 1] - [1 \ 0][1 \ 0] = [0 \ 1] - [0 \ 1] = 0$$

$$[0 \ 1][0 \ 1]$$

From $\textcircled{1}$ and $\textcircled{2}$,

$$\boxed{s_x s_y + s_y s_x = 0}$$

$$\underline{s_x s_y - s_y s_x = i\hbar s_z}$$

$$= \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}$$

$$s_x s_y + s_x s_y = i\hbar s_z$$

$$\Rightarrow \boxed{s_x s_y = \frac{i\hbar s_z}{2}}$$

$$\Rightarrow \frac{1}{2} \frac{\hbar^2}{2} \sigma_x \sigma_y = \frac{i\hbar}{2} s_z = i \frac{\hbar}{2} \frac{\hbar}{2} \sigma_2$$

$$\Rightarrow \boxed{\sigma_x \sigma_y = i \sigma_2}$$

$$\boxed{\sigma_x \sigma_y \sigma_2 = i[I]_{2 \times 2}}$$

$$\sigma_2 = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

To determine eigen values of matrix

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

$$\sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$

$$\sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$|\sigma_x - \lambda_x I| = 0$$

$$|\sigma_y - \lambda_y I| = 0$$

$$|\sigma_z - \lambda_z I| = 0$$

$$\Rightarrow \begin{vmatrix} -\lambda_x & 1 \\ 1 & -\lambda_x \end{vmatrix} = 0$$

$$\Rightarrow \begin{vmatrix} -\lambda_y & -i \\ i & -\lambda_y \end{vmatrix} = 0$$

$$\begin{vmatrix} 1-\lambda_z & 0 \\ 0 & (-1-\lambda_z) \end{vmatrix}$$

$$\Rightarrow \lambda_x^2 - 1 = 0$$

$$\Rightarrow \lambda_y^2 + 1 = 0$$

$$\Rightarrow (1-\lambda_z)(1+\lambda_z) = 0$$

$$\Rightarrow \underline{\lambda_x = \pm 1}$$

$$\Rightarrow \underline{\lambda_y = \pm i}$$

$$\Rightarrow \underline{\lambda_z = \pm 1}$$

~~To find eigen vectors of σ_x~~ for s_x, s_y, s_z

(Coming back to Q-16)

$$\langle x | s_x | x \rangle = \langle x | s_x x \rangle = [x]^T [s_x] [x]$$

$$= [-3i \ 4] \left| \frac{1}{2} \right. \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \left| \begin{bmatrix} 3i \\ 4 \end{bmatrix} \right.$$

$$= \frac{1}{2} \begin{bmatrix} 4 & -3i \end{bmatrix} \left| \begin{bmatrix} 3i \\ 4 \end{bmatrix} \right. \text{ Note that} \\ \text{matrix multiplication} \\ \text{is associative...}$$

$$= \frac{1}{2} \cdot 0 = 0$$

$$\langle x | s_x^2 | x \rangle$$

$$= [-3i \ 4] \frac{1}{2} \lambda^2 \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \left[\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \right] \begin{bmatrix} 3i \\ 4 \end{bmatrix}$$

$$= \frac{25}{4} \lambda^2$$

$$\Rightarrow \Delta s_x = \sqrt{\frac{25}{4} \lambda^2} = \underline{\frac{5}{2} \lambda}$$

$$\begin{array}{ll}
 \textcircled{17} \quad (5, 5, 4) \Rightarrow g_1 = 3 & \\
 (8, 1, 1) \Rightarrow g_2 = 3 & \\
 (7, 4, 1) \qquad \qquad \qquad g_3 = 6 &
 \end{array}
 \left. \right\} \text{Spin is not considered.}$$

General Wave Function of Spin be

$$\chi = \alpha X_{(+)} + \beta X_{(-)}$$

We can write χ as $\begin{bmatrix} \alpha \\ \beta \end{bmatrix}$ with $X_{(+)} = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$ & $X_{(-)} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$

Basis vectors

Let us take general operator S

$$\begin{aligned}
 S(\chi) &= \alpha \underbrace{S(X_{(+)})}_{\downarrow} + \beta \underbrace{S(X_{(-)})}_{\downarrow} \\
 &= \alpha c_1 X_{(+)} + \beta c_2 X_{(-)} \quad (\text{say}) \\
 &= \alpha' X_{(+)} + \beta' X_{(-)} \\
 &= \chi' \quad (\text{say})
 \end{aligned}$$

Now we can write χ' as $\begin{bmatrix} \alpha' \\ \beta' \end{bmatrix}$

What are α' and β'

$$\begin{aligned}
 \underline{\alpha'} &= \langle X_{(+)} | \chi' \rangle \quad \& \quad \underline{\beta} = \langle X_{(-)} | \chi' \rangle \\
 &= \langle X_{(+)} | \alpha S(X_{(+)}) + \beta S(X_{(-)}) \rangle \\
 &= \alpha \langle X_{(+)} | S(X_{(+)}) \rangle + \beta \langle X_{(+)} | S(X_{(-)}) \rangle \\
 &= \underline{\alpha \langle X_{(+)} | S | X_{(+)} \rangle + \beta \langle X_{(+)} | S | X_{(-)} \rangle}
 \end{aligned}$$

Similarly

$$\begin{aligned}
 \underline{\beta'} &= \langle X_{(-)} | \chi' \rangle = \langle X_{(-)} | \alpha S(X_{(+)}) + \beta S(X_{(-)}) \rangle \\
 &= \underline{\alpha \langle X_{(-)} | S | X_{(+)} \rangle + \beta \langle X_{(-)} | S | X_{(+)} \rangle}
 \end{aligned}$$

$$\text{Now } X' = \begin{bmatrix} \alpha \\ \beta \end{bmatrix}$$

$$= \begin{bmatrix} \alpha \langle X_{(+)} | S | X_{(+)} \rangle + \beta \langle X_{(+)} | S | X_{(-)} \rangle \\ \alpha \langle X_{(-)} | S | X_{(+)} \rangle + \beta \langle X_{(-)} | S | X_{(-)} \rangle \end{bmatrix}$$

$$= \begin{bmatrix} \langle X_{(+)} | S | X_{(+)} \rangle & \langle X_{(+)} | S | X_{(-)} \rangle \\ \langle X_{(-)} | S | X_{(+)} \rangle & \langle X_{(-)} | S | X_{(-)} \rangle \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix}$$

$$= S \begin{bmatrix} \alpha \\ \beta \end{bmatrix}$$

$$\Rightarrow S = \boxed{\begin{bmatrix} \langle X_{(+)} | S | X_{(+)} \rangle & \langle X_{(+)} | S | X_{(-)} \rangle \\ \langle X_{(-)} | S | X_{(+)} \rangle & \langle X_{(-)} | S | X_{(-)} \rangle \end{bmatrix}}$$

Note that I can write

$$\vec{\sigma} = \sigma_x \hat{i} + \sigma_y \hat{j} + \sigma_z \hat{k}$$

$$\begin{aligned} \vec{S} &= \frac{1}{2} \hbar \vec{\sigma} = \frac{1}{2} \hbar \sigma_x \hat{i} + \frac{1}{2} \hbar \sigma_y \hat{j} + \frac{1}{2} \hbar \sigma_z \hat{k} \\ &= S_x \hat{i} + S_y \hat{j} + S_z \hat{k} \end{aligned}$$

$$\boxed{\vec{\sigma} \times \vec{\sigma} = 2i \vec{\sigma}}$$

(1) Anti-commutation

$$(2) \sigma_x \sigma_y - \sigma_y \sigma_x = 2i \sigma_z$$

$$(3) \det(\sigma_i) = -1$$

$$(4) \sigma_i^2 = \mathbf{I}$$

$$(5) \sigma_x \sigma_y \sigma_z = i \mathbf{I}$$

$$(6) \text{Tran}(\sigma_i) = 0$$

Properties of Pauli matrices

Since eigenvalues of S_x, S_y, S_z are $\frac{1}{2}\hbar \Rightarrow$ Angular Momentum of spin in any direction can take $(\frac{1}{2})$ value and $|S| = \sqrt{\frac{3\hbar^2}{4}}$

So Basically, let the wave function be

$$|\Psi\rangle = \sum c_i |\phi_i\rangle \quad \text{eg. } \begin{bmatrix} c_1 \\ c_2 \\ c_3 \end{bmatrix}$$

Now applying an operator A upon $|\Psi\rangle$, whose eigenfunctions are $|\phi_i\rangle$'s

$$\begin{aligned} A|\Psi\rangle &= \sum c_i A|\phi_i\rangle \\ &= \sum c_i \lambda_i |\phi_i\rangle \\ &= \sum \lambda'_i |\phi_i\rangle \end{aligned}$$

Hence, new matrix is

$$\begin{bmatrix} \lambda'_1 \\ \lambda'_2 \\ \lambda'_3 \end{bmatrix}$$

Now,

$$\begin{aligned} \lambda'_i &= \langle \phi_i | A|\Psi\rangle \\ &= \langle \phi_i | \sum_j c_j A|\phi_j\rangle \\ &= \sum_j c_j \langle \phi_i | A|\phi_j\rangle \end{aligned}$$

Now this is a matrix representation,

$$\begin{bmatrix} \lambda'_1 \\ \lambda'_2 \\ \lambda'_3 \end{bmatrix} = \begin{bmatrix} \langle \phi_1 | A | \phi_1 \rangle & \langle \phi_1 | A | \phi_2 \rangle & \langle \phi_1 | A | \phi_3 \rangle \\ \langle \phi_2 | A | \phi_1 \rangle & \langle \phi_2 | A | \phi_2 \rangle & \langle \phi_2 | A | \phi_3 \rangle \\ \langle \phi_3 | A | \phi_1 \rangle & \langle \phi_3 | A | \phi_2 \rangle & \langle \phi_3 | A | \phi_3 \rangle \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ c_3 \end{bmatrix}$$

Quantum Physics (12)

Free e⁻ theory of metals

We have done

density of state, $g(E) = \frac{dN(E)}{dE}$

$$\Rightarrow dN(E) = g(E) dE$$

$$\nearrow N(E) = \int dN(E) = \int_0^E g(E) dE$$

Total no. of states = Total no. of states

For fermions, due to spin, 2 particles per state

if $s = \frac{1}{2}$

$$\text{no. of cells} \downarrow \quad \text{no. of particles per cell} \downarrow$$

$$\Rightarrow N = 2 \int_0^{E_f} g(E) f(E) dE$$

Total no. of particles

$$g(E) = \frac{2\pi V}{h^3} (2m)^{\frac{3}{2}} E^{\frac{1}{2}}$$

① $T=0$, $f(E) = 1$ for $E < E_f$.

$$N = 2 \int_0^{E_f} 1 \cdot \frac{2\pi V}{h^3} (2m)^{\frac{3}{2}} \cancel{E^{\frac{1}{2}}} \cancel{dE} E^{\frac{1}{2}} dE$$

$$\therefore \Rightarrow N = \frac{4\pi V}{h^3} (2m)^{\frac{3}{2}} E_f^{\frac{3}{2}} \frac{2}{3}$$

$$E_f = \frac{\hbar^2}{2m} (3\pi^2 n)^{\frac{2}{3}}$$

★ There is a difference in the 2 Ns. Hence the factor of $f(E)$.

Total energy $E = E dN$

$$\Rightarrow E_T = \frac{4\pi V}{h^3} (2m)^{\frac{3}{2}} \int_0^{E_f} E^{\frac{3}{2}} dE = \frac{3}{2} N E_f^{\frac{5}{2}}$$

$$\Rightarrow E_T = \frac{3}{5} N E_f$$

We have calculated $g(\epsilon) d\epsilon$ as

$$\boxed{g(\epsilon) d\epsilon = \frac{d^3 r d^3 p}{h^3}}$$

Now we will derive $g(\epsilon) d\epsilon$ from Quantum Physics.

Atom made of Nucleus and Electrons. We are interested in valency electrons of metal atoms. Due to valency electrons, they are conducting. We say conducting by measuring conductivity ($\sigma = \frac{1}{\rho}$)

Ions will create attractive field. We have to consider motion of electrons in this field.

By suitable choice of scale, we can choose $V=0$

Assuming the state of motion of free electrons as cubical box.

For their motion, $H\psi = E\psi$

In cubical box, we know

$$E = (n_x^2 + n_y^2 + n_z^2) \frac{h^2}{8mL^2}$$

$$\text{Now } n_x^2 + n_y^2 + n_z^2 = \left(\frac{8mL^2}{h^2} E \right) = R^2 \text{ (say)}$$

$$\begin{aligned} dN &= \text{No. of energy states between } E \text{ and } E + dE \\ &= \text{No. of states between } (n_x + dn_x), (n_y + dn_y), \\ &\quad (n_z + dn_z) \end{aligned}$$

$$= \frac{1}{8} \cdot 4\pi R^2 dR$$

$$= \frac{1}{8} \cdot 4\pi \frac{8mL^2}{h^2} E \cdot \sqrt{\frac{8mL^2}{h^2}} \frac{1}{2} \sqrt{E} dE$$

$$dN = \frac{2\pi V}{h^3} (2m)^{\frac{3}{2}} E^{\frac{1}{2}} dE$$

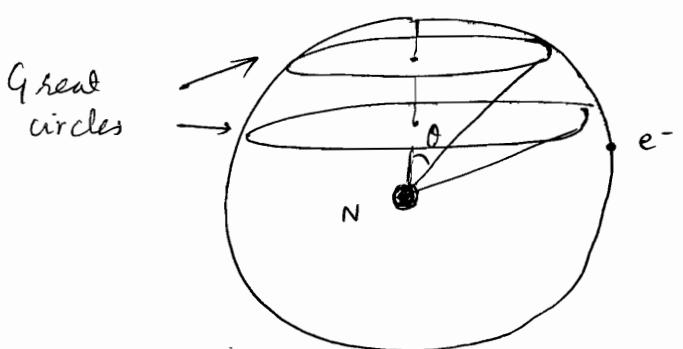
$$\Rightarrow g(\epsilon) d\epsilon = \frac{2\pi V}{h^3} (2m)^{\frac{3}{2}} E^{\frac{1}{2}}$$

• Rest of the analysis is same.

Aim was to derive $g(\epsilon) d\epsilon$ classically as well as Quantum Mechanically !!

Hydrogen Atom Problem

Hydrogen is the simplest atom.



$$V(r), 0 < \theta < \pi$$

$$V(\theta), 0 < \phi < 2\pi$$

$V(\theta)$: we have 1 great circle

$V(\theta)$: we have 1 value of L

Motion corresponding to ϕ gives m .

$$H(\psi) = E(\psi)$$

$$H = \frac{p^2}{2m} + V$$

Frame of Reference = Centre of Mass

$$\Rightarrow \mu = \frac{m_p m_e}{m_p + m_e} = \frac{m_e}{1 + \frac{m_e}{m_p}} \approx m_e$$

Similarly Centre of Mass corresponds to center of nucleus.

$$H = \frac{p^2}{2\mu} + V = -\frac{k^2 \nabla^2}{2me} + V(r)$$

$$V(r) = \frac{-e^2}{4\pi\epsilon_0 r}$$

$$\left(\frac{-\hbar^2}{2\mu} \nabla^2 + V(r) \right) \psi = E \psi$$

$$\Rightarrow \nabla^2 \psi + \frac{2\mu}{\hbar^2} (E - V) \psi = 0$$

Now,

$$\nabla^2 \psi = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial \psi}{\partial r} \right) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \psi}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \left(\frac{\partial^2 \psi}{\partial \phi^2} \right)$$

$$\text{Put } \psi(r, \theta, \phi) = R(r) \Theta(\theta) \Phi(\phi)$$

$$\Rightarrow \oplus \Phi \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial R}{\partial r} \right) + \frac{R \Phi}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left[\sin \theta \frac{\partial \Theta}{\partial \theta} \right] + \frac{R \Theta}{r^2 \sin^2 \theta} \left(\frac{\partial^2 \Phi}{\partial \phi^2} \right) + \frac{2\mu}{\hbar^2} (E - V) R \Theta \Phi = 0$$

$$\Rightarrow \text{Multiply by } \frac{r^2 \sin^2 \theta}{R \Theta \Phi}$$

$$\Rightarrow \frac{\sin^2 \theta}{R} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) + \cancel{\Theta} \frac{\sin \theta}{\Theta} \frac{d}{d\theta} \left(\sin \theta \frac{d\Theta}{d\theta} \right) + \frac{1}{\Phi} \left(\frac{\partial^2 \Phi}{\partial \phi^2} \right) + \frac{2\mu r^2 \sin^2 \theta}{\hbar^2} (E - V) = 0$$

$\underbrace{\quad}_{\text{separate it out by taking it on RHS}}$

$$\Rightarrow \frac{\sin^2 \theta}{R} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) + \frac{2\mu r^2 \sin^2 \theta}{\hbar^2} (E - V) = m^2 - \frac{\sin \theta}{\Theta} \frac{d}{d\theta} \left(\sin \theta \frac{d\Theta}{d\theta} \right)$$

dividing by $\sin^2 \theta$

$$\Rightarrow \frac{1}{R} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) + \frac{2\mu r^2}{\hbar^2} (E - V) = \frac{m^2}{\sin^2 \theta} - \frac{1}{\Theta \sin \theta} \frac{d}{d\theta} \left(\sin \theta \frac{d\Theta}{d\theta} \right)$$

$$f_1(r) = f_2(\theta) = \lambda \text{ (say)}$$

$$\Rightarrow \frac{m^2}{r \sin^2 \theta} - \frac{1}{\theta \sin \theta} \frac{d}{d\theta} \left(\sin \theta \frac{d\Theta}{d\theta} \right) = \lambda$$

$$\text{Let } \cos \theta = x$$

$$\Rightarrow (1-x^2) \frac{d^2 \Theta}{dx^2} - 2x \left(\frac{d\Theta}{dx} \right) + \left(\lambda - \frac{m^2}{1-x^2} \right) \Theta = 0$$

It is associated Legendre's Equation.

$$\text{Solutions are: } \lambda = l(l+1)$$

$$|m| < l$$

$$\Theta = B P_e^m (\cos \theta)$$

where $P_e^m(x)$ are associated Legendre's Polynomials

We have already solved,

$$\Phi = A e^{im\phi}$$

$$\Rightarrow \boxed{\Psi(r, \theta, \phi) = R(r) Y_e^{ml}(\theta, \phi)}$$

Till this point
solution is same
as for Angular Momentum

Motion ϕ fixes m_l : and gives L_z

Motion wrt. θ fixes l : and gives $|\vec{L}| = \sqrt{l(l+1)}$

Motion wrt. r fixes 'n': and gives E

Now our aim is to obtain $R(r)$

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

$$\Rightarrow \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) + \frac{2\mu r^2}{\hbar^2} \left[E - V - \frac{l(l+1)}{2\mu r^2} \hbar^2 \right] R=0$$

Let $V_{eff} = V + \underbrace{\frac{l(l+1)}{2\mu r^2} \hbar^2}_{\text{Centrifugal distortion}}$

Eqn 20.3. of
Neema

Let $\frac{R(r)}{r} = \left(\frac{u(r)}{r} \right)$ and put $r = kr$

$$\Rightarrow \frac{1}{r} \frac{d^2 u}{dr^2} + \frac{2\mu r^2}{\hbar^2} (E - V_{eff}) u_r = 0$$

Solutions of this differential equation are

$$\frac{d^2 u}{dp^2} = k^2 p$$

$$u(p) = A e^{kp} + A e^{-kp}$$

$$\text{as } r \rightarrow \infty, p \rightarrow \infty \Rightarrow u(p) = A e^{-kp}$$

For better solution,

$$u(r) = v(p) u(p)$$

$$v(p) = \sum_{l=0}^{\infty} a_l p^l$$

Series will terminate at $n = j + l + 1$

where l is any integer.
 j is any integer.

$$n_{\min} = 1$$

$$R(r) = R_n(r) : \text{Laguerre's Polynomials}$$

$$E_n = \frac{\hbar^2 k^2}{2}$$

Substituting k ,

$$E_n = -\frac{\mu e^4}{8\epsilon_0^2 c h^3} \frac{1}{n^2} = -\frac{13.6 \text{ eV}}{n^2}$$

define

$$R = \frac{\mu e^4}{8\epsilon_0^2 c h^3}$$

$$E_n = -\frac{Rhc}{n^2}$$

= Rydberg's
Const.

No. restriction on $n^2 \Rightarrow \underline{1 \leq n < \infty}$

$$\begin{aligned} \Rightarrow \Psi(r, \theta, \phi) &= R_n^l \Theta_l^m \Phi^m \\ &= R_n^l P_l^m(\cos\theta) e^{im\phi} \end{aligned}$$

✓ $E_n = -\frac{Rhc}{n^2}$

where $R = \frac{\mu e^4}{8\epsilon_0^2 c h^3}$

$$= -\frac{13.6}{n^2} \text{ eV}$$

$$= 1.09 \times 10^7 \text{ m}^{-1}$$

Q6

$$\boxed{\Psi(n, l, m)}$$

$$\Psi_{n,l,m}(r,0) = \frac{1}{\sqrt{4}} [2 \Psi_{100}(r) - 3 \Psi_{200}(r) + \Psi_{322}(r)]$$

(i) $P = \left(\frac{9}{14}\right) \quad \langle \phi_i | \Psi \rangle^2 = |c_i|^2$

(ii) $\langle H \rangle = \frac{4}{14} \langle 100 | H | 100 \rangle + \frac{9}{14} \langle 200 | H | 200 \rangle + \frac{1}{14} \langle 322 | H | 322 \rangle$

$$= \frac{4}{14} \cdot \left(-\frac{13.6}{1}\right) + \frac{9}{14} \left(-\frac{13.6}{4}\right) + \frac{1}{14} \left(-\frac{13.6}{9}\right)$$

$$\langle L_z \rangle = m_e \hbar$$

$$\langle L_z \rangle = \langle n, l, m_l | L_z | n, l, m_l \rangle \\ = \frac{1}{14} 2\hbar = \left(\frac{\hbar}{7}\right)$$

Q4 $P(r) dr = \Psi^*(r) \Psi(r) 4\pi r^2 dr$

$$\Psi(r) = \frac{1}{\sqrt{\pi}} a^{\frac{3}{2}} e^{-\left(\frac{r}{a}\right)}$$

$$\int_0^\infty P(r) dr = 1 \rightarrow \frac{4\pi}{\pi a^3} \int_0^\infty r^2 e^{-\left(\frac{r}{a}\right)} dr = 1$$

$$\int_0^\infty e^{-x} x^{n-1} dx = \sqrt{n} \rightarrow \frac{4\pi}{\pi a^3} a^2 a \int_0^\infty x^2 e^{-x} dx = \text{Put } \frac{r}{a} = x$$

$$P(r) = \frac{4\pi}{\pi a^3} e^{-\frac{2r}{a}} r^2$$

Maximum at $\left. \frac{dP(r)}{dr} \right|_{r=r_{\min}} = 0$

$$\left. \frac{d^2 P(r)}{dr^2} \right|_{r=r_{\min}} < 0$$

$$e^{-\frac{2r}{a}} (2r) + r^2 \left(e^{-\frac{2r}{a}} \right) \cdot \left(\frac{2}{a} \right) = 0$$

$\Rightarrow r = a$ *

Also Note,

$$\psi_{(100)} = \psi_{(1s)} \quad \begin{array}{l} n_{\min} = 1 \\ l_{\min} = 0 \end{array}$$

$$\psi_{(200)} = \psi_{(2s)} \quad \begin{array}{l} \text{For given } n, \text{ there are } n \\ \text{values of } l, \end{array}$$

$$\psi_{(210)} = \psi_{(2p_x)} \quad [0, 1, 2, \dots, n-1]$$

$$\psi_{(211)} = \psi_{(2p_y)}$$

For each l , $(2l+1)$ values of m_l

$$\psi_{(212)} = \psi_{(2p_z)}$$

Also for every n , 2 spin

$(2, 8, 18, \dots)$ remember shell configuration!!

\Rightarrow For a given E_n , $\frac{2n^2}{2 \sum (2l+1)} = 2n^2$ degenerate states

$\circ n=1$: ground state

$$\Psi_{(1,00)} = \frac{1}{\sqrt{\pi} a^{3/2}} e^{-\frac{r}{a}}$$

| |
|---|
| a : Bohr Radius $= \frac{(4\pi\epsilon_0 \hbar^2)}{(mee^2)}$ $= 0.53 \text{ \AA}$ |
|---|

$$\langle r^n \rangle = \int_0^\infty \left(\frac{1}{\sqrt{\pi} a^{3/2}} e^{-\frac{r}{a}} \right)^n r^n \frac{1}{\sqrt{\pi} a^{3/2}} e^{-\frac{r}{a}} dr$$

$$= \frac{4}{a^3} \int_0^\infty r^{n+2} e^{-\frac{2r}{a}} dr$$

$$= \frac{4}{a^3} \left(\frac{a}{2} \right)^{n+3} \int_0^\infty x^{n+2} e^{-x} dx$$

$$\frac{2r}{a} = x$$

$$= \frac{1}{a^3} \left(\frac{a}{2}\right)^{n+3} \sqrt{n+3}$$

$$\boxed{\langle r^n \rangle = \frac{1}{2} \left(\frac{a}{2}\right)^n \sqrt{n+3}}$$

in ground state $\Psi(1,0,0)$

$$\langle r \rangle = \frac{1}{2} \frac{a}{2} \sqrt{4} = \frac{1}{4} a \cdot L_3 = \left(\frac{3a}{2}\right)$$

$$\langle \frac{1}{r} \rangle = \frac{1}{2} \left(\frac{a}{2}\right)^1 \sqrt{2} = \left(\frac{1}{a}\right)$$

$$\boxed{4\pi e^2 : \frac{HcI}{2mc^2}}$$

$$\langle r^2 \rangle = \frac{1}{2} \left(\frac{a}{2}\right)^2 \sqrt{5} = \frac{4 \cdot 3 \cdot 2}{8} \frac{a^2}{2} = 3a^2$$

$$\downarrow \quad \langle \mathbf{r}^n \rangle = \langle n, l, m | r^n | n, l, m \rangle$$

$$d\tau = r^2 \sin \theta \ dr d\theta d\phi$$

$$\langle V \rangle = -\frac{e^2}{4\pi\epsilon_0} \langle \frac{1}{r} \rangle$$

$$\langle E \rangle = \langle n | H | n \rangle = -\frac{13.6}{n^2} \text{ eV}$$

$$\boxed{\langle T \rangle = \langle E \rangle - \langle V \rangle}$$

do not do
by any other
method

<https://ourstudycircle.in/upscpdf/>

Quantum Mechanics (13)

19/02/2022

For any dynamical variable, rate of change of its expectation value is given by

$$\boxed{\frac{d}{dt} \langle a \rangle = \frac{1}{i\hbar} \langle [a, H] \rangle + \langle \frac{\partial a}{\partial t} \rangle}$$

Heisenberg's
theorem

e.g. ② $\frac{\partial}{\partial t} \langle p_x \rangle = \frac{1}{i\hbar} \langle [p_x, H] \rangle + 0$ } [Because p_x is not a function of time]

$$① \frac{\partial}{\partial t} \langle x \rangle = \frac{1}{i\hbar} \langle [x, H] \rangle$$

Application of
Heisenberg's Theorem

Description of motion of
particle in quantum mechanics

From ① $\frac{\partial}{\partial t} \langle x \rangle = \frac{1}{i\hbar} \langle [x, H] \rangle$

$$= \frac{1}{i\hbar} \langle \left[x, \frac{p_x^2}{2m} + V(x) \right] \rangle$$

$$= \frac{1}{i\hbar} \langle \left[x, \frac{p_x^2}{2m} \right] \rangle + \frac{1}{i\hbar} \langle [x, V(x)] \rangle$$

$$= \frac{1}{i2m\hbar} \langle [x, p_x^2] \rangle$$

$$x (-i\hbar)^2 \frac{\partial^2 \psi}{\partial x^2}$$

$$= \frac{1}{i2m\hbar} 2i\hbar p_x$$

$$+ (-i\hbar)^2 \frac{\partial^2 (x\psi)}{\partial x^2}$$

$$= \left[\frac{\langle p_x \rangle}{m} \right]$$

$$= - \frac{(-i\hbar)^2 \partial^2}{m}$$

From ② ,

$$\begin{aligned}\frac{\partial \langle p_x \rangle}{\partial t} &= \frac{1}{i\hbar} \langle [p_x, H] \rangle \\&= \frac{1}{i\hbar} \left\langle \left[p_x, \frac{p_x^2}{2m} \right] \right\rangle + \frac{1}{i\hbar} \langle [p_x, v_x] \rangle \\&= \frac{1}{i\hbar} \langle [p_x, v_x] \rangle \quad [p_x, v_x] \psi \\&= \frac{1}{i\hbar} \left\langle i\hbar \left(\frac{\partial v_x}{\partial x} \right) \right\rangle \\&= \left\langle -\frac{\partial V}{\partial x} \right\rangle \quad -i\hbar \frac{\partial (\psi)}{\partial x} - i\hbar \psi \left(\frac{\partial V}{\partial x} \right) \\&= - \left\langle \frac{\partial V}{\partial x} \right\rangle \quad = -i\hbar \left(\frac{\partial V}{\partial x} \right) \psi\end{aligned}$$

If operator A for any dynamical variable 'a' is not an explicit function of time . then $\langle \frac{\partial A}{\partial t} \rangle = 0$

$$\Rightarrow \frac{d}{dt} \langle a \rangle = \frac{1}{i\hbar} \langle [A, H] \rangle$$

If 'a' is a const. of motion $\Rightarrow \frac{1}{i\hbar} \langle [A, H] \rangle = 0$

or

If $[A, H] = 0 \Rightarrow 'a' \text{ is a const. of motion}$

Eg. for free particle,

$$[P_x, H] = [P_x, \frac{P_x^2}{2m}] = 0$$

$\Rightarrow \langle P_x \rangle$ is a const. of motion.

$$\Rightarrow \frac{\partial \langle P_x \rangle}{\partial t} = \frac{1}{i\hbar} \langle [P_x, H] \rangle = 0 \therefore \underline{\underline{\langle P_x \rangle = \text{const.}}}$$

→ Prove that
for a
free
particle
momentum
is a const. of
motion.

Derivation of $\therefore \frac{d}{dt} \langle a \rangle = \frac{1}{i\hbar} \langle [A, H] \rangle + \langle \frac{\partial A}{\partial t} \rangle$

$$\langle a \rangle = \langle \psi | A | \psi \rangle$$

$$\frac{d}{dt} \langle a \rangle = \langle \psi | A | \left(\frac{\partial \psi}{\partial t} \right) \rangle + \underbrace{\langle \psi | \frac{\partial A}{\partial t} | \psi \rangle}_{= \langle \frac{\partial A}{\partial t} \rangle} + \langle \frac{\partial \psi}{\partial t} | A | \psi \rangle$$

$$\Rightarrow \frac{d}{dt} \langle a \rangle = \langle \psi | A | \frac{\partial \psi}{\partial t} \rangle + \langle \frac{\partial \psi}{\partial t} | A | \psi \rangle + \langle \frac{\partial A}{\partial t} \rangle$$

$$H\psi = i\hbar \left(\frac{\partial \psi}{\partial t} \right) \quad \dots \quad \text{Time dependent Schrodinger wave}$$

Note that time dependent Schrodinger Eqn is the only source of time derivatives of ψ !!

$$\Rightarrow \frac{d}{dt} \langle a \rangle = \frac{1}{i\hbar} \langle \psi | A | H\psi \rangle + \langle \frac{\partial \psi}{\partial t} | A | \psi \rangle$$

$$-\frac{1}{i\hbar} \langle \psi | H$$

$$+ \frac{1}{i\hbar} H\psi = \left(\frac{\partial \psi}{\partial t} \right) \Rightarrow -\frac{1}{i\hbar} \psi^* H = \frac{\partial \psi^*}{\partial t} = \langle \frac{\partial \psi}{\partial t} |$$

$$\Rightarrow \frac{d}{dt} \langle a \rangle = \frac{1}{i\hbar} \langle \psi | A H | \psi \rangle - \frac{1}{i\hbar} \langle \psi | H A | \psi \rangle$$

(Using H is Hermitian)

$$\frac{d}{dt} \langle a \rangle = \frac{1}{i\hbar} \left[\langle \psi | A H | \psi \rangle - \langle \psi | H A | \psi \rangle \right] + \langle \frac{\partial A}{\partial t} \rangle$$

$$\frac{\partial}{\partial t} \langle a \rangle = \frac{1}{i\hbar} \langle [A, H] \rangle + \langle \frac{\partial A}{\partial t} \rangle$$

$\star \boxed{\langle A \rangle \Leftrightarrow \langle \psi | A | \psi \rangle} = \langle a \rangle$

Parabolic Potential Well (from advanced Quantum Mechanics)

We know

$$L_{(+)} |l, m\rangle = \sqrt{(l-m)(l+m+1)} \quad \nparallel \quad |l, m+1\rangle$$

$$L_{(-)} |l, m\rangle = \sqrt{(l+m)(l-m+1)} \quad \nparallel \quad |l, m-1\rangle$$

$$L_x = \frac{L_{(+)} + L_{(-)}}{2}$$

$$L_y = \frac{L_{(+)} - L_{(-)}}{2i}$$

From Harmonic Oscillator, we know

$$E_n = \left(n + \frac{1}{2}\right) \hbar \omega$$

$$\psi_n = C_n H_n(x) e^{-\frac{m\omega x^2}{2\hbar}}$$

Let us introduce another operator $a_{(-)}$, s.t.

$$a_{(-)} \psi_0 = 0$$

$$a_{(-)} \psi_n = C_1 \psi_{(n-1)}$$

$a_{(-)}$: Step down Operator

$$\boxed{a_{(-)} |n\rangle = C_1 |n-1\rangle}$$

$$\boxed{C_1 = \sqrt{n}}$$

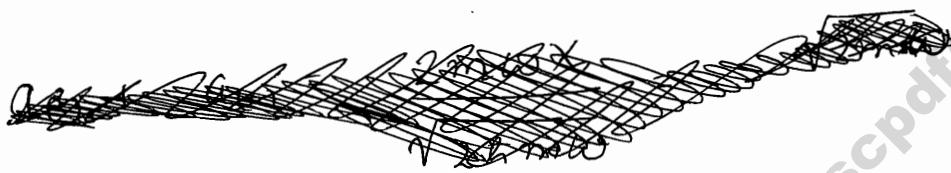
Correspondingly,

$$a_{(+)} |n\rangle = c_2 |n+1\rangle$$

$$c_2 = \sqrt{n+1}$$

$a_{(+)}$: Step up operator

$$\begin{aligned} a_{(+)} &= (m\omega X - i^{\circ}P_x) \frac{1}{\sqrt{2\hbar m\omega}} \\ a_{(-)} &= (m\omega X + i^{\circ}P_x) \frac{1}{\sqrt{2\hbar m\omega}} \end{aligned}$$



$$\begin{aligned} a_{(+)} a_{(-)} &= \frac{1}{2\hbar m\omega} ((m\omega X - i^{\circ}P_x)(m\omega X + i^{\circ}P_x)) \\ &= \frac{1}{2\hbar m\omega} (m^2\omega^2 X^2 + im\omega(XP_x - P_x X) + P_x^2) \\ &= \frac{1}{\hbar\omega} \left(\frac{P_x^2}{2m} + \frac{1}{2} m\omega^2 X^2 + \frac{i\omega}{2} (i\hbar) \right) \\ &= \frac{1}{\hbar\omega} \left(H - \frac{\hbar\omega}{2} \right) \end{aligned}$$

$$a_{(+)} a_{(-)} = \left(\frac{H}{\hbar\omega} - \frac{1}{2} \right)$$

$\Rightarrow a_{(+)} a_{(-)}$: Pure Number

$$\Rightarrow \hbar\omega \left(a_{(+)} a_{(-)} + \frac{1}{2} \right) = H$$

Similarly

$$[a_{(-)}, a_{(+)}] = \frac{\hbar}{m\omega} + \frac{1}{2}$$

$$\Rightarrow H = \hbar\omega \left(a_{(-)} a_{(+)} - \frac{1}{2} \right)$$

$$\Rightarrow a_{(+)} a_{(-)} - a_{(-)} a_{(+)} = -1$$

$$\Rightarrow [a_{(+)}, a_{(-)}] = -1$$

Note that we can find X, P_x ,
of $a_{(+)}$ and $a_{(-)}$.

$$\text{eg. } X = \frac{\sqrt{2\hbar m\omega}}{2m\omega} (a_{(+)} + a_{(-)})$$

$$= \sqrt{\frac{\hbar}{2m\omega}} (a_{(+)} + a_{(-)})$$

$$P_x = \frac{\sqrt{2\hbar m\omega}}{2m\omega} (a_{(+)} - a_{(-)})$$

$$= i\sqrt{\frac{\hbar m\omega}{2}} (a_{(+)} - a_{(-)})$$

- define : ① a_+ , a_-
- ② $N = a_+ a_-$ (define)
- ③ $|n\rangle$ as eigen function of N with eigen value n . (a number)
- ④ $[N a_+] = a_+$
using $[a_+ a_-] = -1$
 $[a_- a_+] = 1$

$$⑤ [N a_-] = -a_-$$

$$⑥ N[a_{+n}] = (n+1)|n\rangle$$

$$\Rightarrow a_{+|n\rangle} = C_1 |n+1\rangle$$

$$⑦ N[a_{-|n\rangle}] = (n-1) a_{-|n\rangle}$$

$$-1 \Rightarrow a_{-|n\rangle} = C_2 |n-1\rangle$$

$$⑧ \text{Using norm}$$

$$\langle n | a_{+|n+1\rangle} = |a_+|^2$$

$$\langle n | N+1 | n \rangle = |a_+|^2$$

$$|a_+|^2 = \sqrt{n+1}$$

$$⑨ \langle n | a_{+a_-|n\rangle} = |a_+|^2$$

$$|a_+|^2 = \sqrt{n}$$

H in terms

$$⑩ a_{-|0\rangle} = 0$$

$$⑪ \text{Prove } \begin{cases} n \geq 0 \\ n \in \mathbb{Z} \end{cases}$$

Continuously
apply $a_{(-)}$

for $n \in (0, 1)$

$$a_{-|n\rangle} = \sqrt{n} |n-1\rangle$$

eigenvalue $(n-1)$
not possible to
be negative

Now, what is their importance?

$$\psi_n(x) = C_n H_n(x) e^{-\frac{m\omega}{2\hbar} x^2}$$

Find $\langle T_n \rangle$ and $\langle V_n \rangle$

or

Prove $\langle T_n \rangle = \left(n + \frac{1}{2}\right) \frac{\hbar\omega}{2}$

& $\langle V_n \rangle = \left(n + \frac{1}{2}\right) \frac{\hbar\omega}{2}$

$$\begin{aligned}\langle V_n \rangle &= \frac{1}{2} m \omega^2 \langle x^2 \rangle \\ &= \frac{1}{2} m \omega^2 | \psi_n | x^2 | \psi_n | \end{aligned}$$

Now we can write x^2 in terms of $a(+)$ and $a(-)$

Similarly for k.E., we can write $E_n - \langle V_n \rangle = \langle T_n \rangle$
To calculate E_0

$$H\psi = E\psi$$

$$H_0\psi_0 = E_0\psi_0$$

$$\hbar\omega (a_{-}, a_{+}, \psi_0) - \frac{1}{2} \hbar\omega \psi_0$$

$$\hbar\omega (a_{-}) \sqrt{1} \psi_1 - \frac{1}{2} \hbar\omega \psi_0$$

$$= \hbar\omega (\sqrt{1} \sqrt{1} \cdot \psi_0) - \frac{1}{2} \hbar\omega \psi_0$$

$$= \frac{1}{2} \hbar\omega \psi_0$$

$$\Rightarrow E_0 = \frac{1}{2} \hbar\omega$$

To calculate ψ_0

$$\text{Now } a_{+} \psi_0 = 0$$

$$\Rightarrow \frac{1}{\sqrt{2\hbar m\omega}} (iP_x + m\omega X) \psi_0 = 0$$

$$\Rightarrow i(-i\hbar \frac{\partial \psi_0}{\partial x}) + m\omega x \psi_0 = 0$$

$$\Rightarrow \cancel{i} \frac{\partial \psi_0}{\partial x} = -\left(\frac{m\omega x}{\hbar}\right) \psi_0$$

$$\Rightarrow \int \frac{d\psi_0}{d\psi_0} = -\frac{m\omega}{\hbar} \int x dx$$

$$\Rightarrow \boxed{\psi_0 = A e^{-\left(\frac{m\omega x^2}{2\hbar}\right)}}$$

$$\langle \psi_0 | \psi_0 \rangle = 1$$
$$\Rightarrow \boxed{A = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}}}$$

$$a_{+} |\psi_0\rangle = |\psi_1\rangle$$

$$a_{+} |\psi_1\rangle = \sqrt{2} |\psi_2\rangle$$

To find ψ_1

$$\Rightarrow \psi_1 = a_{+} |\psi_0\rangle$$

$$= \frac{1}{\sqrt{2\hbar m\omega}} [-iP_x + m\omega X] \left[\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{m\omega x^2}{2\hbar}}\right]$$

$$= \frac{2m\omega \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}}}{\sqrt{2\hbar m\omega}} x e^{-\left(\frac{m\omega x^2}{2\hbar}\right)}$$

$$H\psi_1 = E\psi_1$$

To find E

$$\hbar\omega \left(a_{(-)} a_{(+)} - \frac{1}{2} \right) \psi_1$$

$$= \hbar\omega \left(a_{(-)} a_{(+)} \psi_1 - \frac{1}{2} \psi_1 \right)$$

$$= \hbar\omega \left(\sqrt{2} \sqrt{2} \psi_1 - \frac{1}{2} \psi_1 \right)$$

$$= \frac{3}{2} \hbar\omega \psi_1$$

$$\Rightarrow \boxed{E = \frac{3}{2} \hbar\omega}$$

Or write
 $a_{-} a_{+} = N^{+1}$
 $\hbar\omega (N^{1m}) + \hbar\omega^{1m} - \frac{1}{2} \hbar\omega^{1m}$
 ~~$\hbar\omega^{1m} + \frac{\hbar\omega}{2} m$~~
 ~~$(N^{+1}) \hbar\omega m$~~

Q) We know in $\psi_n(x) = C_n H_n(x) e^{-\left(\frac{m\omega}{2\hbar}\right)x^2}$

Prove HUP

$$\Delta x \Delta p_x \geq \frac{\hbar}{2}$$

& find out $\langle T \rangle$, $\langle V \rangle$ and $\langle H \rangle$

A) We need to find out only $\langle x^2 \rangle$ and $\langle p_x^2 \rangle$
 $\langle x \rangle$ and $\langle p_x \rangle$

$$\langle T \rangle = \frac{\langle p_x^2 \rangle}{2m}$$

$$\langle V \rangle = \frac{1}{2} m \omega^2 \langle x^2 \rangle$$

$$\langle H \rangle = \langle T \rangle + \langle V \rangle$$

NOTE THAT I
DO NOT REQUIRE
WAVE FUNCTION !!

$$X = \sqrt{\frac{\hbar}{2m\omega}} (a_{(+)} + a_{(-)})$$

$$X^2 = \left(\sqrt{\frac{\hbar}{2m\omega}} \right)^2 (a_{(+)}^2 + a_{(-)}^2 + a_{(+)} a_{(-)} + a_{(-)} a_{(+)})$$

$$= \frac{\hbar}{2m\omega} (a_{(+)}^2 + a_{(-)}^2 + 2a_{(-)}a_{(+)} + 1)$$

$$\langle n | x | n \rangle = \sqrt{\frac{\hbar}{2m\omega}} \langle n | a_{(+)} + a_{(-)} | n \rangle$$

$$= \sqrt{\frac{\hbar}{2m\omega}} \langle n | \sqrt{n+1} | n+1 \rangle + \sqrt{\frac{\hbar}{2m\omega}} \langle n | \sqrt{n} | n-1 \rangle$$

$$= 0 + 0$$

$$= 0$$

$$\langle n | x^2 | n \rangle$$

they will vanish

\downarrow

$$= \frac{\hbar}{2m\omega} \langle n | a_{(+)}^2 + a_{(-)}^2 + 2a_{(-)}a_{(+)} + 1 | n \rangle$$

$$= \frac{\hbar}{2m\omega} \langle n | 2a_{(-)}a_{(+)} + 1 | n \rangle$$

$$= \frac{\hbar}{m\omega} \langle n | a_{(+)}a_{(+)} | n \rangle + \frac{\hbar}{2m\omega} \langle n | n \rangle$$

$$= \frac{\hbar}{m\omega} \langle n | a_{(-)}\sqrt{n+1} | n+1 \rangle - \frac{\hbar}{2m\omega} \langle n | n \rangle$$

$$= \frac{(\sqrt{n+1})^2 \hbar}{m\omega} \langle n | n \rangle + \frac{\hbar}{2m\omega} \langle n | n \rangle$$

$$= \left[(n+1) + \frac{1}{2} \right] \frac{\hbar}{m\omega}$$

$$= \left(n + \frac{1}{2} \right) \frac{\hbar}{m\omega}$$

$$\langle V \rangle = \frac{1}{2} m \omega^2 \langle n^2 \rangle$$

$$= \frac{1}{2} m \omega^2 (2n+1) \frac{\hbar \omega}{2m \omega}$$

$$\boxed{\langle V_n \rangle = \frac{\hbar \omega}{2} \left(n + \frac{1}{2}\right)}$$

Similarly using $\langle P_x \rangle$, $\langle P_{x^2} \rangle$, we can find

$$\boxed{\langle T_n \rangle = \frac{\hbar \omega}{2} \left(n + \frac{1}{2}\right)}.$$

Q10) $\psi(x, y, z) = \sqrt{\frac{8}{L^3}} \sin\left(\frac{\pi x}{L}\right) \sin\left(\frac{\pi y}{L}\right) \sin\left(\frac{\pi z}{L}\right)$

Find $\langle p_x \rangle$, $\langle p_{x^2} \rangle$ in $0 < x < L$

$$\begin{aligned} \langle \psi | \psi \rangle &= \frac{8}{L^3} \int_0^L \int_0^L \int_0^L \sin^2\left(\frac{\pi x}{L}\right) \sin^2\left(\frac{\pi y}{L}\right) \sin^2\left(\frac{\pi z}{L}\right) dx dy dz \\ &= \frac{8}{L^3} \int \int \left(\frac{L}{2}\right) \sin^2\left(\frac{\pi y}{L}\right) \sin^2\left(\frac{\pi z}{L}\right) dy dz \\ &= \frac{8}{L^3} \cdot \frac{L^3}{8} = 1 \end{aligned}$$

$$\langle p_x \rangle = \frac{\langle \psi | P_x | \psi \rangle}{\langle \psi | \psi \rangle} = \langle \psi | P_x | \psi \rangle$$

$$\langle p_{x^2} \rangle = \frac{\langle \psi | P_{x^2} | \psi \rangle}{\langle \psi | \psi \rangle} = \langle \psi | P_{x^2} | \psi \rangle$$

$$\langle \psi | p_x | \psi \rangle = \langle \psi | -i\hbar \frac{\partial}{\partial x} \psi \rangle$$

$$= -i\hbar \iiint \psi^*(x, y, z) \frac{\partial \psi}{\partial x} dx dy dz$$

$$= -i\hbar \int_0^L \int_0^L \int_0^L \left(\frac{8}{L^3} \right) \sin\left(\frac{\pi x}{L}\right) \sin^2\left(\frac{\pi y}{L}\right) \sin^2\left(\frac{\pi z}{L}\right) \cos\left(\frac{\pi x}{L}\right) dx dy dz$$

$$= \frac{\pi - i\hbar^4}{L^3} \int_0^L \underbrace{\sin \frac{2\pi x}{L}}_{dx} \int_0^L \sin^2\left(\frac{\pi y}{L}\right) dy \int_0^L \sin^2\left(\frac{\pi z}{L}\right) dz$$

$$= 0$$

① Note that we cannot write $\Psi(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{\pi x}{L}\right)$
 IT IS COMPLETELY WRONG !!

$$\langle \psi | p_x^2 | \psi \rangle = \langle \psi | -\hbar^2 \frac{\partial^2}{\partial x^2} \psi \rangle$$

$$= -\hbar^2 \iiint \frac{8}{L^3} \sin \frac{\pi x}{L} \sin^2 \frac{\pi y}{L} \sin^2 \frac{\pi z}{L} \frac{\pi^2}{L^2} \sin \frac{\pi x}{L} dx dy dz$$

$$= -\hbar^2 \frac{\pi^2}{L^2} \frac{8}{L^3} \int_0^L \sin^2 \frac{\pi x}{L} dx \int_0^L \sin^2 \left(\frac{\pi y}{L} \right) dy \int_0^L \sin^2 \left(\frac{\pi z}{L} \right) dz$$

$$= \left(\frac{\pi \hbar}{L} \right)^2 \frac{8}{L^3} \left(\frac{L}{2} \cdot \frac{L}{2} \cdot \frac{L}{2} \right)$$

$$= \left(\frac{\hbar^2}{4L^2} \right)$$

Q 21)

$$\psi(x) = C_1 \phi_1(x) + C_2 \phi_2(x)$$

$$\phi_n(x) = \sqrt{\frac{2}{a}} \sin\left(\frac{n\pi x}{a}\right)$$

$$\begin{aligned} \psi(x) &= C \sqrt{\frac{a}{2}} \sqrt{\frac{2}{a}} \sin\left(\frac{\pi x}{a}\right) + \frac{C}{2} \sqrt{\frac{a}{2}} \sqrt{\frac{2}{a}} \sin\left(\frac{2\pi x}{a}\right) \\ &= C \sqrt{\frac{a}{2}} \phi_1(x) + \frac{C\sqrt{a}}{2\sqrt{2}} \phi_2(x) \end{aligned}$$

$$\langle \psi | \psi \rangle = 1$$

$$C^2 \frac{a}{2} + \frac{C^2 a}{8} = 1$$

$$C = \underline{\underline{\sqrt{\frac{8}{5a}}}}$$

* Important thing is to write $\psi(x)$ as $C_1 \phi_1(x) + C_2 \phi_2(x)$ where C_1 and C_2 are free numbers.

$$\Rightarrow \psi(x) = \sqrt{\frac{8}{5a}} \sin\left(\frac{\pi x}{a}\right) + \sqrt{\frac{2}{5a}} \sin\left(\frac{2\pi x}{a}\right)$$

$$= \sqrt{\frac{4}{5}} \phi_1(x) + \sqrt{\frac{1}{5}} \phi_2(x)$$

$\langle E \rangle$

$$= \langle \psi | H | \psi \rangle$$

$$= \cancel{\langle \psi | \phi_1 | \phi_1 \rangle} \frac{4}{5} \langle \phi_1 | H | \phi_1 \rangle + \frac{1}{5} \langle \phi_2 | H | \phi_2 \rangle$$

$$\langle n | H | n \rangle = m^2 \frac{\hbar^2}{8ma^2}$$

$$\Rightarrow \frac{4}{5} \cdot \left(\frac{\hbar^2}{8ma^2} \right) + \frac{1}{5} \cdot 4 \cdot \left(\frac{\hbar^2}{8ma^2} \right) = \underline{\underline{\frac{\hbar^2}{5ma^2}}}$$

$$\textcircled{1} \quad P_i = |c_i|^2 = |\langle \phi_i | \psi \rangle|^2 \quad \text{if } \psi = \sum c_i \phi_i$$

Q An e⁻ is given in $|l, m\rangle = \frac{1}{\sqrt{14}} Y_3^0 + \frac{2}{\sqrt{14}} \cdot Y_3^{-1}$

Find $\langle L^2 \rangle, \langle L_z \rangle$
 $\langle S_z \rangle, \langle S_z^2 \rangle, \langle \mu_b \rangle$

$$+ \frac{3}{\sqrt{14}} Y_2^2$$

We can see $\langle l, m | l, m \rangle = 1$

F.

$$\langle l, m | L^2 | l, m \rangle = l(l+1) \hbar^2$$

$$\langle l, m | L_z | l, m \rangle = m \hbar$$

$$\langle l, m | L^2 | l, m \rangle = \frac{1}{14} \langle 3, 0 | L^2 | 3, 0 \rangle \quad \textcircled{12}$$

$$+ \frac{4}{14} \langle 3, +1 | L^2 | 3, -1 \rangle \quad \textcircled{13}$$

$$+ \frac{9}{14} \langle 2, 2 | L^2 | 2, 2 \rangle \quad \textcircled{14}$$

$$= \left(\frac{104}{14} \right) \hbar^2 \quad \checkmark$$

$$\langle l, m | L_z | l, m \rangle$$

$$= \frac{1}{14} \cdot 0 + \frac{4}{14} \cdot (-1\ h) + \frac{9}{14} \cdot (2\ h)$$

$$= \cancel{\frac{1}{14}} \checkmark$$

$$\vec{\mu} = \vec{\mu}_L + \vec{\mu}_S$$

$$= -\frac{e}{2m} (\vec{L} + 2\vec{S})$$

$$\mu_z = -\frac{e}{2m} (L_z + 2S_z)$$

$$\langle \mu_z \rangle = -\frac{e}{2m} (\langle L_z \rangle + 2\langle S_z \rangle)$$

$$= -\frac{e\ h}{2m} + \frac{e}{m} \langle S_z \rangle$$

$$S_z = m_s \ h = \pm \frac{1}{2} \ h$$

$$\langle S_z \rangle = \langle s, m | S_z | s, m \rangle$$

Wave Function has no relation with spin.

$$= \langle \chi_+ | S_z | \chi_- \rangle + \langle \chi_- | S_z | \chi_+ \rangle$$

$$|\psi, m\rangle = c_1 \chi_+ + c_2 \chi_- \quad (\text{given if } \chi = \begin{pmatrix} -3/5 \\ 5/4 \end{pmatrix})$$

$$\langle S_z \rangle = |c_1|^2 \langle \chi_+ | S_z | \chi_+ \rangle + |c_2|^2 \langle \chi_- | S_z | \chi_- \rangle$$

$$= \frac{9}{25} \langle \chi_+ | S_z | \chi_+ \rangle + \frac{16}{25} \langle \chi_- | S_z | \chi_- \rangle$$

$$= \frac{9}{25} \frac{1}{2} \hbar \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$= \frac{1}{2} \hbar \frac{9}{25} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$= \frac{1}{2} \hbar \left(\frac{9}{25} \right)$$

+

$$\frac{1}{2} \hbar \frac{16}{25} \begin{bmatrix} 0 & 1 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$= \hbar \frac{8}{25} \begin{bmatrix} 0 & -1 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix}$$

$$= -\hbar \frac{8}{25}$$

$$\langle S_z \rangle = -\frac{7}{50} \hbar$$

Proof of H atom

Step 1 : Complete Equation

$$\frac{1}{r^2} \left(\frac{d}{dr} \left(r^2 \frac{d\psi}{dr} \right) + \frac{1}{r^2 \sin \theta} \frac{d}{d\theta} \left(\sin \theta \frac{d\psi}{d\theta} \right) \right) + \frac{1}{r^2 \sin^2 \theta} \frac{d^2 \psi}{d\phi^2} + \frac{2m}{\hbar^2} \left(E + \frac{e^2}{4\pi\epsilon_0 r} \right) \psi = 0$$

Step 2 : Separate ϕ by multiply by $r^2 \sin^2 \theta$ and writing ψ as $R \Theta \Phi$ and dividing by $R \Theta \Phi$

$$\frac{\sin^2 \theta}{R} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) + \frac{\sin \theta}{\Theta} \frac{d}{d\theta} \left(\sin \theta \frac{d\Theta}{d\theta} \right) + \frac{2m\sigma^2}{\hbar^2} \left(E + \frac{e^2}{4\pi\epsilon_0 r} \right) \sin^2 \theta = -\frac{1}{\Phi} \frac{d^2 \Phi}{d\phi^2} = m^2 \quad (\text{say})$$

$$\boxed{\Phi = A e^{im\phi}}$$

Step 3 : Separate Θ by dividing by $\sin^2 \theta$

$$\frac{1}{R} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) + \frac{2m}{\hbar^2} r^2 \left(E + \frac{e^2}{4\pi\epsilon_0 r} \right) = \left[\frac{m^2}{\sin^2 \theta} - \frac{1}{\sin \theta} \Theta \frac{d}{d\theta} \left(\sin \theta \frac{d\Theta}{d\theta} \right) \right] = l(l+1) \quad (\text{say})$$

$$\boxed{\Theta = P_l^m(\cos \theta)}$$

Step 4 : Write the "r" equation properly by multiplying by R and dividing by r^2

$$\frac{1}{r^2} \frac{d}{dr} \left(r^2 \frac{dR}{dr} \right) + \left[\frac{2mE}{\hbar^2} + \frac{2me^2}{4\pi\epsilon_0 \hbar^2 r} - \frac{l(l+1)}{r^2} \right] R = 0$$

Step 5 : Substitution

let $p = 2kr$ (dimensionless)

$$k = \sqrt{-\frac{2mE}{\hbar^2}} \quad (\text{wave number})$$

$$\lambda = \left(\frac{mc^2}{4\pi\epsilon_0 \hbar^2 k} \right) \quad (\text{dimensionless})$$

replacing and dividing by $4k^2$,

$$\frac{1}{p^2} \frac{d}{dp} \left(p^2 \frac{dR}{dp} \right) + \left[-\frac{1}{4} + \frac{\lambda}{p} - \frac{l(l+1)}{p^2} \right] = 0$$

Step 6 : Asymptotic behaviour

When $p \rightarrow \infty$, i.e. $r \rightarrow \infty$, we have

$$\frac{1}{p^2} \frac{d}{dp} \left(p^2 \frac{dR}{dp} \right) - \frac{R}{4} = 0$$

We'll get $\boxed{R = e^{-\frac{p}{2}}}$

Step 7 : Polynomial function

Let the solution be of form

$$R = e^{-\frac{p}{2}} F(p)$$

where F is a polynomial

$$\Rightarrow \frac{dR}{dp} = -\frac{1}{2} e^{-\frac{p}{2}} F + e^{-\frac{p}{2}} F'$$

$$\Rightarrow \frac{d}{dp} \left(p^2 \frac{dR}{dp} \right) = e^{-\frac{p}{2}} F'' + \left(\frac{2}{p} - 1 \right) e^{-\frac{p}{2}} F' + \left(\frac{1}{4} - \frac{1}{p} \right) e^{-\frac{p}{2}} F$$

Using it in the actual equation,

$$e^{-\frac{p}{2}} \left[p^2 F'' + F' \left[\frac{2}{p} - 1 \right] + F \left[\frac{1}{4} - \frac{1}{p} \right] + \left[-\frac{1}{4} + \frac{\lambda}{p} - \frac{l(l+1)}{p^2} \right] F \right] = 0$$

$$\Rightarrow F'' + F' \left[\frac{2}{p} - 1 \right] + F \left[\frac{\lambda-1}{p} - \frac{l(l+1)}{p^2} \right] = 0$$

Step 8 Use power series to expand

$$\text{let } F(p) = p^s \sum_{j=0}^{\infty} a_j p^j = p^s G(p)$$

where $j, s \in \mathbb{Z}^+$ (positive integers)

otherwise at $s=0$, $F \rightarrow \infty$

This form ensures that F is finite at $p=0$

$$\Rightarrow \sum a_j \left\{ (j+s)(j+s+1) \right\} p^{j+s+2} - l(l+1) \\ - \sum a_j \left\{ (j+s) - (\lambda-1) \right\} p^{s+j-1} = 0$$

Step 9 Separating $j=0$ from 1st term

$$\Rightarrow a_0 \left\{ s(s+1) - l(l+1) \right\} p^{s-2} + \sum_{j=1} a_j \left\{ (j+s)(j+s+1) - l(l+1) \right\} p^{j+s-2} \\ - \sum_{j=0} a_j \left\{ (j+s) - (\lambda-1) \right\} p^{j+s-1} = 0$$

Put $j = j' + 1$

$$\Rightarrow a_0 \left\{ s(s+1) - l(l+1) \right\} p^{s-2} + \sum_{j'=0} a_{j'+1} \left\{ (j'+s+1)(j'+s+2) - l(l+1) \right\} p^{j'+s-1} \\ + \sum_{j=0} a_j \left\{ (j+s) - (\lambda-1) \right\} p^{j+s-1} = 0$$

Replacing j' by j as
it's just a symbol for
summation, we have

$$a_0 \left(s(s+1) - l(l+1) \right) p^{s-2} + \sum_j \left(a_{j+1} \left[(j+s+1)(j+s+2) - l(l+1) \right] - a_j \left[(j+s) - (\lambda-1) \right] \right) p^{s+j-1} = 0$$

Step 10 Putting Coefficient = 0

If $A + Bx + Cx^2 = 0$
for all x

$$\Rightarrow A = B = C = 0$$

\therefore we have

$$s(s+1) - l(l+1) = 0$$

$$\Rightarrow s = l \quad \text{or} \quad s = -(l+1)$$

$$\Rightarrow s = l$$

$$s \in \mathbb{Z}^+$$

$$[(j+s+1)(j+s+2) - \ell(\ell+1)] \alpha_{j+1} - \alpha_j [(j+s) - (\lambda-1)] = 0$$

$$\Rightarrow \frac{\alpha_{j+1}}{\alpha_j} = \frac{(j+\ell) - (\lambda-1)}{(j+\ell+1)(j+\ell+2) - \ell(\ell+1)}$$

Step 11 Termination/
Truncation for some
power of j

$$j_{\max} + \ell - \lambda + 1 = 0$$

$$\Rightarrow \lambda = j_{\max} + \ell + 1 = n \text{ (say)}$$

$$\therefore n \in \mathbb{Z} \Rightarrow \lambda \in \mathbb{Z}$$

$$\Rightarrow \lambda = \ell+1, \ell+2, \ell+3, \dots = n$$

$$\text{Now } \lambda = \frac{m^2 e^2}{4\pi \epsilon_0 \hbar^2 k} \text{ and } k = \sqrt{\frac{2mE}{\hbar^2}}$$

$$\Rightarrow n^2 = -\frac{m^2 e^4}{(4\pi \epsilon_0)^2 \hbar^2 2mE} \frac{\hbar^2}{k^2}$$

$$\Rightarrow E = -\frac{m e^4}{2 (4\pi \epsilon_0)^2 \hbar^2 n^2}$$

$$= -\left(\frac{13.6}{n^2}\right)eV$$

Step 12 Eigen Function

Put $F = p^\ell G(p)$, we get

$$F'' = p^\ell G'' + 2\ell p^{\ell-1} G' + \ell(\ell-1)p^{\ell-2} G$$

$$F'\left(\frac{2}{p} - 1\right) = G''(2p^{\ell-1} - p^\ell) + G(2\ell p^{\ell-2} - \ell p^{\ell-1})$$

$$F\left[\frac{2}{p} - \frac{\ell(\ell+1)}{p^2}\right] = G[(\lambda-1)p^{\ell-1} - \ell(\ell+1)p^\ell]$$

Step 13 divide by $p^{\ell-1}$ and
combine $(2\ell+1)$, we get

$$p G'' + ((2\ell+1)+1-p) G' + [(n+\ell) - (2\ell+1)] G = 0$$

This is precisely the
Associated Laguerre Equation,
whose solution is

$$G(p) = C L_{n+\ell}^{2\ell+1}(p)$$

$$\text{where } L_{n+\ell}^{2\ell+1} = \frac{d^{2\ell+1}}{dp^{2\ell+1}} (L_{n+\ell})$$

is called Associated Laguerre
Polynomial

$$\& L_n(p) = e^p \frac{d^n}{dp^n} (p^n e^{-p})$$

Ques 14 Replace ρ

$$\text{Now } \rho = \left(\frac{2Zr}{na_0} \right)$$

where $a_0 = \text{bohr radius}$

$$= \left(\frac{4\pi \epsilon_0 h^2}{me^2} \right)$$

$$\Rightarrow R(\rho) = C e^{-\frac{\rho}{a_0}} \rho^l L_{n+l}^{2l+1}(\rho)$$

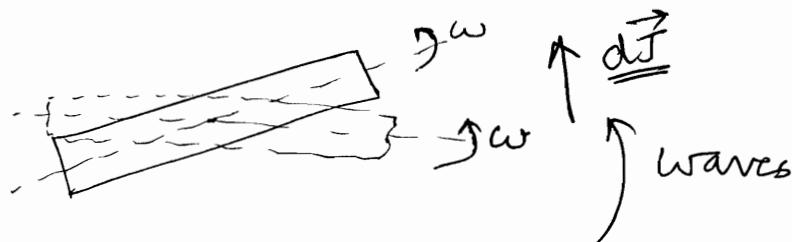
$$= C e^{-\frac{Zr}{na_0}} \left(\frac{2Zr}{na_0} \right)^l L_{n+l}^{2l+1} \left(\frac{2Zr}{na_0} \right)$$

For $n=1, l=0, m=0$

$$\Psi_1 = \frac{1}{\sqrt{\pi}} \cdot \left(\frac{Z}{a_0} \right)^{\frac{3}{2}} e^{-\frac{Zr}{a_0}}$$



but if



⇒ Similarly



Bullet motion spiral type due to grooves in bullet

It ensures better & accurate motion.
Spin of the bullet provided by "rifling" (screw type structure of the gun barrel), gyroscopically stabilizes the bullet.

④ P-49 Ans: $\sqrt{\frac{2N_0 a^2}{m}}$

Method-1 $\sqrt{\frac{1}{m} \left(\frac{d^2 V}{dx^2} \right)}$

Method-2 Open $V(r)$ in form of Taylor expansion, ignore higher power of $(r-r_0)$

④ P-54 : ①

④ R-88

④ I-90

④ P-97

④ R-98 ④ R-102

④ P-12 (II)
14 (Bound states)

④ P-78