Physics - 5

Matrix Multiplication

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

[as long as you preserve the order]

- Complex Conjugate or Conjugate Matrix :- complex conjugate of each element.

$$A_1 = \bar{A}$$

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

(for Hermitian Operators)

(*) Proof of Heisenbergs : end of lecture 2

(*) Proof of H atom : end of notes

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days	Lectures	Chapters (Verma)
2	1	1, 2, 3
	2	4, 5
3	3, 4	6, 7, 8, 9, 10, 11
	5	12
	6, 7, 8, 13	13, 14, 15, 16, 17
2	9, 10, 11	18, 19
	12	20, 21

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

- $(\nabla^2 + k^2)\,\frac{e^{ikr}}{r} = -4\pi\,\delta(\vec{r})$

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

- define $\delta(r - r') = \delta(x-x')\cdot\delta(y-y')\cdot\delta(z-z')$

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

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

1) Basic Concepts (Preliminaries)
   - Wave Particle duality
   - Heisenberg's Uncertainty Principle
   - Axioms of Quantum Mechanics

     (Eigen Values, 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

(iv) Rectangular Barrier

(v) Simple Harmonic Oscillator

(vi) H atom problem

3) E.V. problem of Angular Momentum Measurement

- Orbital Angular Momentum
- Spin Angular Momentum (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 <u>Principle of Complimentarity</u>

Wave Particle Duality

Debroglie's Concept of Material Waves

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

$$\boxed{E^2 = (pc)^2 + (m_0c^2)^2}$$

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

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

$$\Rightarrow \underbrace{p}_{\text{particle property}} = \frac{h\nu}{c} = \underbrace{\left(\frac{h}{\lambda}\right)}_{\text{wave property}} \Rightarrow \boxed{\lambda = \left(\frac{h}{p}\right)}$$

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

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

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

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

⊛ hypothesis $\xrightarrow[\text{verification}]{\text{experimental}}$ theory

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

(non-relativistic energy)

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

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

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

Q/ λ of neutron at 300k $= \dfrac{h}{\sqrt{3mkT}}$ (since $f=3$) $\boxed{\text{For thermal neutron, } f=2}$

Q/ Energy of $e^- =$ 1 keV $\lambda = \dfrac{h}{\sqrt{2mE}}$

Energy of $e^- =$ 1 MeV $\boxed{\lambda = \frac{hc}{pc} = \frac{hc}{\sqrt{E^2 - (m_o c^2)^2}}}$

(Since $E >$ rest mass energy, it is Relativistic Energy)

[For e^- : $m_o c^2 = 0.51$ MeV]

Q/ λ cricket Ball

assuming critical Ball to be particle

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

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

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)

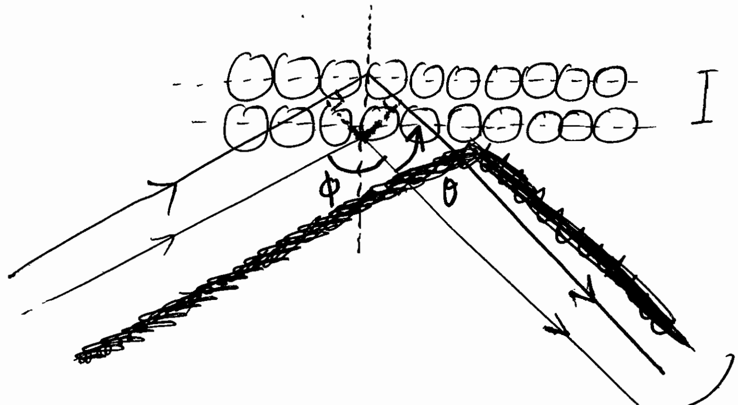
$$\lambda = \frac{h}{mv} = \frac{6.62 \times 10^{-34}}{9.1 \times 10^{-31} \times 10^6} \simeq 7.3 \times 10^{-10} \text{ m} \approx \underline{7 \text{ Å}}$$

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. Laue had diffraction of X-rays made possible using crystal arrangement of atoms.

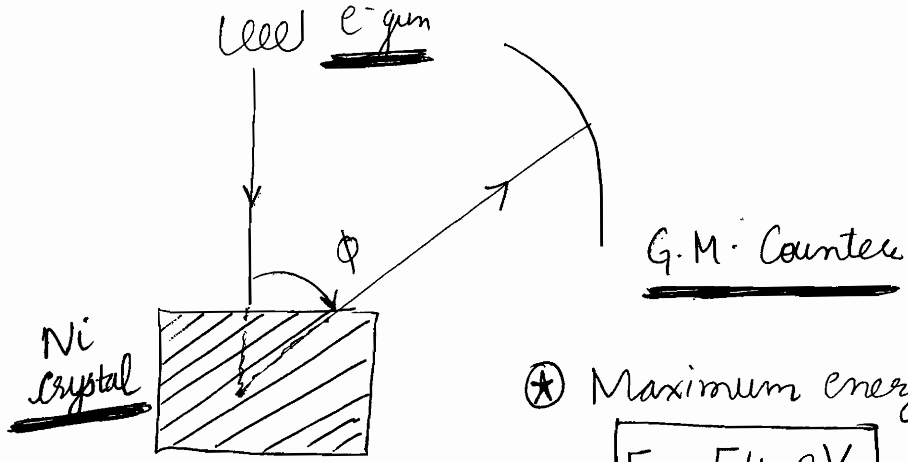


I $d \approx \lambda_{X\text{-ray}}$ [Inter Planar Spacing]

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

intensity maximum at what angle of diffraction at what incident energy.

⊙ Garibaldi (1850) : unification of Italy
⊙ Grimaldi (1650) : diffraction



(*) Maximum energy/intensity observed for,

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

Assuming validity of wave-particle duality:

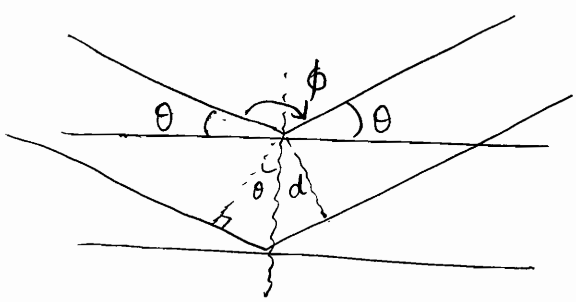
$$\lambda = \frac{h}{\sqrt{2mE}}$$

$$= \frac{6.6\times10^{-34}}{\sqrt{2\times 9.1\times10^{-31}\times 54\times 1.6\times10^{-19}}} \qquad = 1.66\,\text{Å}$$

$$= \frac{6.6\times10^{-34}}{9.49\times\cancel{10^{-3}}\times10^{-25}}$$

$$= 0.166\times10^{-9}$$

Bragg's law for diffraction



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

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

For 1st Maxima,

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

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

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

For Ni Crystal: $d = 0.92\,\text{Å}$

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

$$= 1.66\,\text{Å}$$

Hence λ comes out to be same. Hence wave-particle duality confirmed for electrons.

We know

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

valid

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

(for material waves)

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

* 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

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

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

$$v_g = \frac{d\omega}{dk} = \frac{\hbar\, d\omega}{\hbar\, dk} = \frac{dE}{dp} = \frac{c^2 p}{E} = \frac{c^2 \cancel{m} v}{mc^2} = v$$

$$\boxed{E^2 = p^2c^2 + (m_0c^2)^2 \Rightarrow 2E\, dE = 2pc^2\, dp}$$

$$\Rightarrow \boxed{v_g = v}$$

→ 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.

Note that it points towards HUP

We can also write,

$$\boxed{\lambda = \frac{h}{p} = \frac{hc}{\sqrt{T^2 + 2T m_0 c^2}}}$$

$$\boxed{(T + m_0c^2)^2 = (pc)^2 + (m_0c^2)^2}$$

Total expression

$$= \frac{\frac{1}{2}m_0v^2 + m_0c^2}{mv}$$

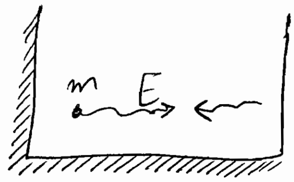
$$= \frac{c^2}{v}\left[\frac{m_0 + \frac{m_0}{2}\frac{v^2}{c^2}}{m}\right]$$

$$\approx \left(\frac{c^2}{v}\right)$$

1-d Box

$\Downarrow$

Motion in a straight line

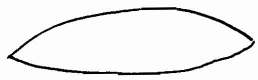


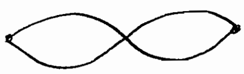
$L = (\lambda/2)$

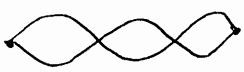
$\rightarrow$ Quantization of energy is inherent in De Broglie's theory

$$E = \frac{p^2}{2m}$$ (non relativistic)

Standing Waves will form.

$L = \frac{\lambda}{2}$  No hindranace

$L = \frac{2\lambda}{2}$  1 hindrance

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

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

⊙ Note that we can observe HOP from here $\Delta p . \Delta x \leq \frac{h}{2L} . L \leq \left(\frac{h}{2}\right)$

$\rightarrow$ n cannot be 0 (Momentum is discrete)

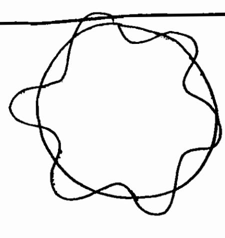
$$p_n = \frac{h}{\lambda_n} = \frac{nh}{2L}$$

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

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

⊙ Hence, particle in a box executing 1-d motion, cannot have any value of Energy. It can have only discrete values of E
$E = n^2\Delta$
where $\Delta = \left(\frac{h^2}{8mL^2}\right)$

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



Remember, for H atom,

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

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

$$L = p . r = \left(\frac{nh}{2\pi}\right)$$ Bohr Quantization of Ang. Momentum

Quantum (2)

7/02/2012

$$\boxed{\begin{aligned} \vec{p} &= \hbar \vec{k} \\ E &= \hbar\omega = mc^2 \end{aligned}}$$

- Canonical Conjugate variables $[q, p_q]$

(position) $x \to P_x$ (momentum)

(general) $q \to P_q$

(lifetime) $t \to E$ (energy)

$\theta \to J$

$$\boxed{x \longleftrightarrow K_x}$$

- <u>Fourier transform</u>

expansion coefficient

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

1-d description

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

बत्ती	$t \to \omega$
फिज़िक्स	$x \to p$

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

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

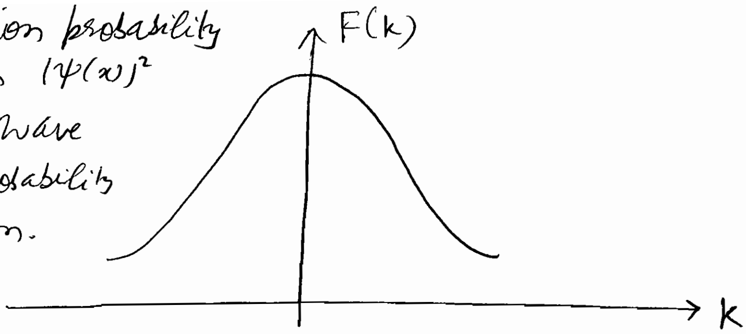
$$\psi(x) = F(x) = \frac{1}{\sqrt{2\pi}} \int f(k)\, e^{ikx}\, dk_x$$

Refer eqn. 4.5, 4.6 of HC-Verma

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

$(p = k\hbar)$

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



An example of F(k)

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

expansion coefficient of moving particle

Fourier transforms of
$x \leftrightarrow k$: no $1/\sqrt{\hbar}$
$x \leftrightarrow p$: $\frac{1}{\sqrt{\hbar}}$ in denominator for proper units

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

3-d description

Gaussian Wave Packet Treatment of free particle

P-65 Verma

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

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

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

Now if k is distributed normally,

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

σ : standard deviation

mean = 0

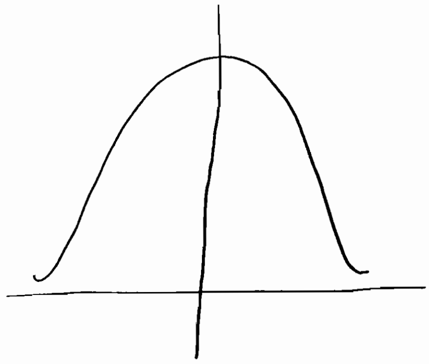
[in general $\quad f(x) = A\, e^{-\frac{(x-x_0)^2}{2\sigma^2}}$: gaussian $dist^n$]

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

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

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

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



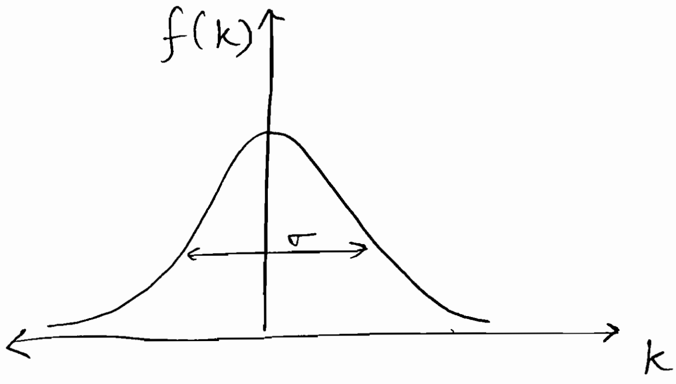
$$\Rightarrow \boxed{\sigma = \sqrt{\langle x^2 \rangle - \langle x \rangle^2}}$$

σ = S.D. is error in measurement of x

$\langle x \rangle$: Expectation Value of x $= \dfrac{\sum x\, f(x)}{\sum f(x)}$ ← Probability $dist^n$

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

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



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

$$= 0$$

$\sigma = \Delta k$: 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

---

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

Gamma Function

$\downarrow$

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

$\Gamma(1) = 1$

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

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

$$\boxed{\int_0^{\infty} e^{-x} x^n\, dx = \Gamma(n+1)}$$

$$\boxed{\int_0^{\infty} x^n e^{-\alpha x^2}\, dx = \frac{1}{2(\alpha)^{\frac{n+1}{2}}}\, \Gamma\left(\frac{n+1}{2}\right)} \quad \begin{matrix}\alpha > 0 \\ n > -1\end{matrix}$$

$$\boxed{\int_{-\infty}^{\infty} e^{-\alpha x^2 \pm \beta x}\, dx = \sqrt{\frac{\pi}{\alpha}}\; e^{\frac{\beta^2}{4\alpha}}} \quad (\alpha > 0)$$

$$\Rightarrow A\sqrt{\frac{\pi\, 2\sigma^2}{1}} = 1 \qquad \Rightarrow \boxed{A = \frac{1}{\sqrt{2\pi}\,\sigma}}$$

(*) Fourier Transform of Gaussian is a Gaussian Function

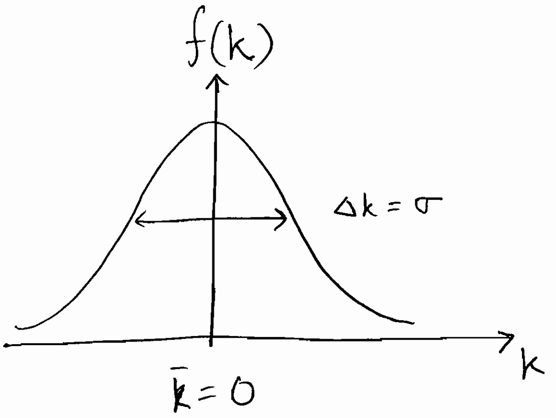
$$F(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} f(k)\, e^{jkx}\, dk$$

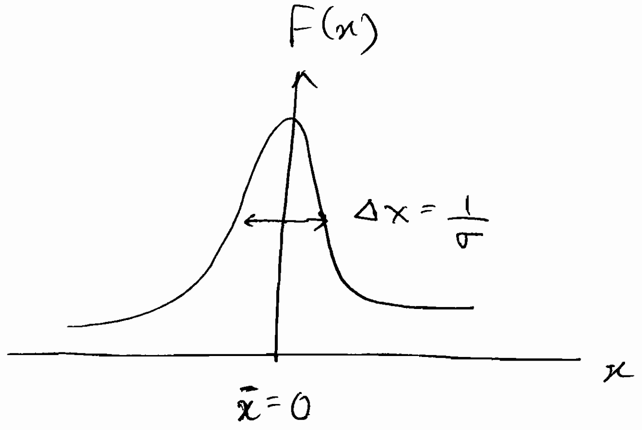
$$= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \frac{1}{\sigma\sqrt{2\pi}}\, e^{-\frac{k^2}{2\sigma^2} + jkx}\, dk$$

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

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

which turns out to be gaussian distⁿ.





$\Delta k = \sigma$

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

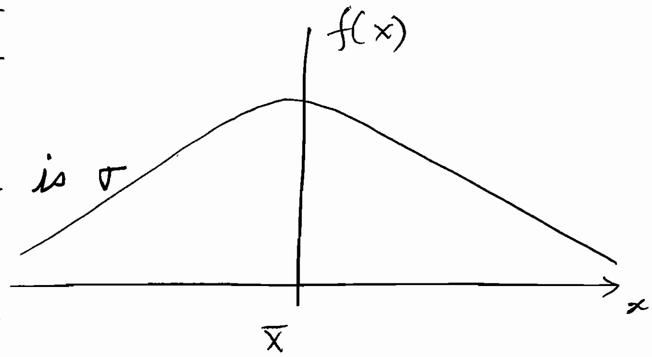
→ Note that Δk can be considered as error in measurement of k or the actual variation of k.

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

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

We can start from $f(x)$ = 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 $\bar{x} = 0$

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

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

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

$$= \sigma^2$$

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

$$= \frac{1}{\sqrt{2\pi}} \int \frac{1}{\sigma\sqrt{2\pi}}\, e^{-\frac{x^2}{2\sigma^2} - ikx}\, dx$$

$$= \frac{1}{\sigma(2\pi)} \sqrt{\frac{\pi\, 2\sigma^2}{\cancel{\alpha}}}\; e^{-\frac{k^2}{4} \cdot 2\cancel{\sigma}^2}$$

$$= \frac{1}{\sqrt{2\pi}}\, e^{-\frac{k^2}{2\left(\frac{1}{\sigma}\right)^2}}$$

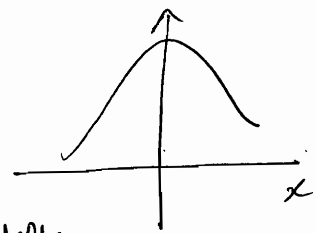
$\Rightarrow \quad \Delta x = \sigma$

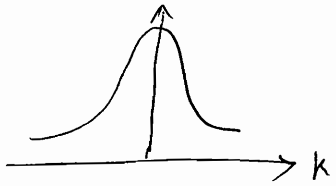
$\Delta k = \frac{1}{\sigma}$

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

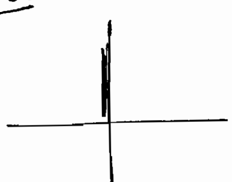
Cannonical Conjugate variables $\qquad \Delta x \; \Delta y = \text{Const.}$

$\Uparrow$ Both cannot be precisely measured simultaneously





<u>dirac delta</u>

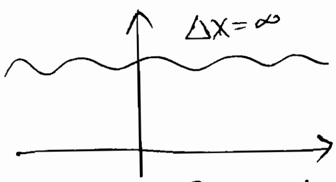


$\Delta x = 0$

$\Delta k = \infty$

<u>plane wave</u>

$\Delta x = \infty$



$\Delta x \approx x$:- Range of $x = \infty$ $\qquad \Delta k = 0 \qquad \Delta k \simeq k$: Range of $k = \infty$

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

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

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

$$= \psi_0\, e^{ikx}\, e^{-i\omega t}$$

$$= \psi_0\, e^{i(kx-\omega t)}$$

Since we always take $e^{-i\omega t}$ $\Rightarrow$ e^{ikx} means wave travelling in positive x direction & $e^{-ikx} \Rightarrow$ negative x dirⁿ

Heisenberg's Uncertainty Principle

Product of errors of 2 Conjugate variables's measurement:

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

Comparing the orders,

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

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

basic heisenberg relationship

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

energetic लोग जल्दी मर जाते हैं !!

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

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

$$\Delta q \, \Delta p_q \geq \frac{\hbar}{2}$$

where

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

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

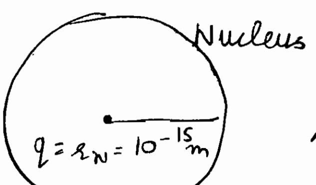
1) e^- cannot reside inside the nucleus. Prove
2) Find out ground state radius & energy of H atom.
3) Find out minimum energy of Harmonic Oscillator i.e. Parabolic Potential Well.
4) Mass of π Meson (exchange particle) is what, when range of interaction is r?
5) Spectral width of any line i.e. $\Delta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

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

$\boxed{e^- \text{ Cannot reside in the nucleus.}}$

Order of Nuclear Potential Well $\approx$ $\boxed{28 - 35 \text{ MeV}}$

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



Position $\rightarrow$ $\Delta q_{max} = 10^{-15}$ m

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

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

Momentum must be comparable with error in momentum

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

(note that it is relativistic energy)

$$E = \sqrt{(pc)^2 + (m_0c^2)^2} \approx pc \qquad [100 \gg 0.51]$$

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

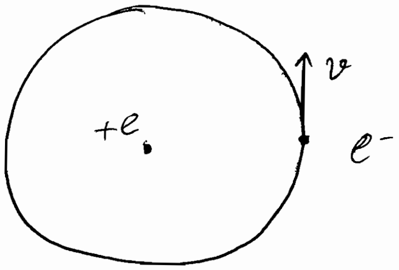
$$= 100 \text{ MeV}$$

We can even put all the values

$$\frac{6.6 \times 3 \times 10^8}{2 \times 2\pi \times 1.6} \simeq 0.98 \times 10 = \underline{\underline{100 \text{ MeV}}}$$

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

$\boxed{\text{H atom}}$ take $(\hbar)$



At r

$$\text{K.E}(r) = \frac{p^2}{2m} - \frac{e^2}{4\pi\epsilon_0 r}$$

We know $\Delta r \Delta p_r \geq \left(\frac{\hbar}{2}\right)$

For minimum energy, $\boxed{\Delta r \ast \Delta p_r \approx \hbar}$

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

$$E(r) = \frac{\hbar^2}{2m_e x^2} - \frac{e^2}{4\pi\epsilon_0 x}.$$

Note that
$m = m_e$

As atom is assumed to be at rest K.E. is possessed by e^- only.

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

⊛ do not use approximations like $\pi^2 = 10$ or $\hbar = 10^{-34}$ as the values are too small s.t. approximation completely changes the answer!!

$\left[\frac{4\pi\epsilon_0 \hbar^2}{me^2}\right]$ $\boxed{r_0 = 0.53\,\text{Å}}$ ✓

$-\frac{me^4}{32\pi^2\epsilon_0^2\hbar^2}$ $\boxed{E_{r_0} = -13.6\,eV}$ ✓

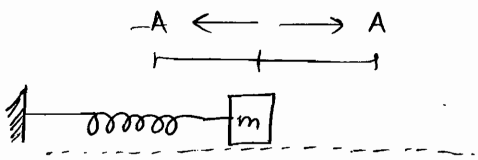
⊛ do not forget $\frac{1}{2\pi}$ in expression of $\hbar$

Simple Harmonic Oscillator : Minimum Energy

Refer Verma : P-67

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

and $\Delta x = \cancel{x}$
$\Delta p = \left(\frac{\hbar}{2x}\right)$



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

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

just to remember

$$\boxed{\Delta x \ \Delta p_x \approx \hbar}$$

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

$$\Delta x = 2A$$

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

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

Put $\frac{dE}{dA} = 0$

$$\frac{-2\hbar^2}{8mA^3} + kA = 0 \Rightarrow A = \sqrt[4]{\frac{2\hbar^2}{8mk}}$$

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

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

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

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

Mass of Exchange Particle $\approx \left(\hbar\right)$

$$\boxed{\Delta E\,\Delta t \approx \hbar}$$

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

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

Spectral Width take $\left(\hbar\right)$

$$E = h\nu \qquad \Delta E\,\Delta t \approx \hbar$$

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

Step 1 **Proof of Heisenberg**

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 $(\Delta X)^2 = \langle X^2 \rangle - \langle X \rangle^2$

$= \langle X'^2 \rangle$ — (1)

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

$= \langle P_x'^2 \rangle$ — (2)

Also $[X', P_x']$

$= [X - \langle x \rangle, P_x - \langle p_x \rangle]$

$= [X, P_x]$ — (3)

Step 3

Let us consider an arbitary 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 $|\psi\rangle$

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

(do not worry about P'^* and we can write $i\hbar\frac{\partial}{\partial x}$ as $\underline{iP}$)

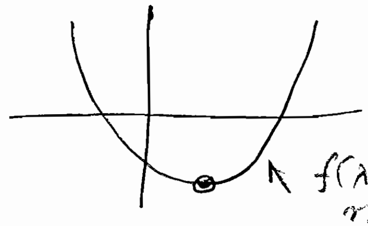
$\Rightarrow \lambda^2\langle P'^2\rangle + \lambda\langle i[X', P']\rangle + \langle X'^2\rangle \geq 0$

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

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

Step 5

Its a parabola in λ with $a > 0$



$f(\lambda) < 0$ not allowed

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

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

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

Put $[X, P] = i\hbar$

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

(in 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,

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

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

Let us take

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

$$g = i x \psi$$

Evaluating the 1st term of LHS

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

$$= \hbar^2 \int_V \frac{\partial \psi^*}{\partial x} \frac{\partial \psi}{\partial x} \, d\tau$$

$$= \hbar^2 \iiint \overset{\mathrm{I}}{\left(\frac{\partial \psi}{\partial x}\right)} \overset{\mathrm{II}}{\left(\frac{\partial \psi}{\partial x}\right)^*} \, dx \, dy \, dz$$

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

$$= \hbar^2 \iint \underbrace{\left[\left(\frac{\partial \psi}{\partial x}\right) \psi^*\right]_{-\infty}^{\infty}}_{=0} dy \, dz \; - \; \hbar^2 \iiint \left(\frac{\partial^2 \psi}{\partial x^2}\right) \psi^* \, dx \, dy \, dz$$

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

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

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

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

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

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

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

$$\int g^* g \, d\tau$$

$$= \int -ix\psi^* \; ix\psi \, d\tau$$

$$= \int \psi^* \psi \, x^2 \, d\tau$$

$$= \langle x^2 \rangle = (\Delta x)^2 \qquad (\text{i.e. } \sigma_x^2)$$

<u>We have taken</u>

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

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

$$g = ix\psi = i \, x \, \psi$$

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

<u>R.H.S</u>

<u>Proof of Heisenberg limit to be Gaussian Function</u>

Wave Function

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

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

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

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

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

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

Also, k and x are cannonical conjugates i.e. both cannot be determined precisely simultaneously.

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

Wave Function

Both can be complex

In this eqn, inbuilt are

- Plank's Quantization
- De Broglie's wave theory
- Heisenberg Uncertainty Principle

Note that Wave Function is not displacement

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 Borne's Explanation of ψ

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

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

$$\frac{dP}{d\tau} \propto \psi^* \psi$$

$$\Rightarrow \boxed{dP \propto \psi^* \psi \, d\tau}$$

$$\text{Probability} \propto \int_V \psi^* \psi \, d\tau$$ ← Hence $\psi(x)$ has units of $\frac{1}{\sqrt{\text{Length}}}$

and $\psi(r)$ has units of $\frac{1}{\sqrt{\text{Volume}}}$

Hence, only $A(k)$ will come in Probability, no part e^{ikx} in calculation of Probability. $[e^{ikx} * e^{-ikx} = 1]$

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

$$\boxed{\text{Prob} \propto \int \psi^*(x) \, \psi(x) \, dx}$$ **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

Total space

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

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

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

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

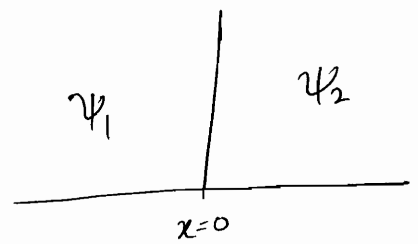
$\psi = e^{kx}$: Not possible as $\psi \to \infty$ as $x \to \infty$

Good Function for $x < 0$

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

$\psi = \sin x$: good function

CONTINUOUS



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

if ~~differentiable~~ $\left(\frac{d\psi_1}{dx}\right) = \left(\frac{d\psi_2}{dx}\right)$ ~~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	$\vec{J} = \vec{r} \times \vec{p}$	$\vec{r} \times -i\hbar\vec{\nabla}$ $= -i\hbar(\vec{r} \times \vec{\nabla})$
④ Energy "E"		$i\hbar\frac{\partial}{\partial t}$

○ Remember from EM

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

$$\boxed{\frac{\partial}{\partial t} \equiv -i\omega} \Rightarrow +i\frac{\partial}{\partial t} = \frac{E}{\hbar} \Rightarrow E = +i\hbar\frac{\partial}{\partial t}$$

---

(5) kinetic Energy $\quad T = \frac{p^2}{2m} \quad\quad -\frac{\hbar^2}{2m}\nabla^2$

(6) Potential Energy $\quad V \quad\quad V$

(7) Mechanical Energy $\quad T+V \quad\quad H$ (Hamiltonian

$$= T+V$$

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

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

(✱)

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

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)

GIST OF QUANTUM THEORY

$$\boxed{a\psi = A\,\psi}$$

hence every dynamical variable is quantized i.e. can have only definite values and not a continuum

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

$$A \psi_n = a_n \psi_n$$

Mathematical Operator

a_n : eigen values

ψ_n : states or eigen functions

$$A \psi_1 = a_1 \psi_1$$

$$A \psi_2 = a_2 \psi_2$$

$$\vdots$$

$$A \psi_n = a_n \psi_n$$

$$\text{Prob} = |\psi_n|^2$$

We also write,

$$\boxed{A \, |\psi\rangle = a \, |\psi\rangle}$$

We had studied in matrices,

$$AX = \lambda X$$

X : eigen functions / vectors

λ : eigen values

Example : ① Measure Momentum p_x

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

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

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

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

[Plane Wave]

② Measure position x

$$x \psi = x_0 \psi$$

$$\Rightarrow \psi = \delta(x - x_0)$$

[Dirac Delta]

Now p_x cannot be imaginary, otherwise ψ can become $\propto$
(anyways, ψ cannot be a as its not square integrable. It can
be eigenfunction ofcourse. wavefunction)

② Measure Energy

$$H\psi_n = E_n\psi_n$$

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

Schrodinger's Wave Equation :

[S 2016]

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

: Time independent form

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

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

③ Angular Momentum :-

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

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

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

$a_n = \{a_1, a_2, \ldots a_n\}$]

⑥ Expectation value or Most representative Value

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

Note that it is discrete

$$\boxed{\langle a \rangle = \frac{\int \psi^* A \psi \, d\tau}{\int \psi^* \psi \, d\tau}}$$

if it is continuous

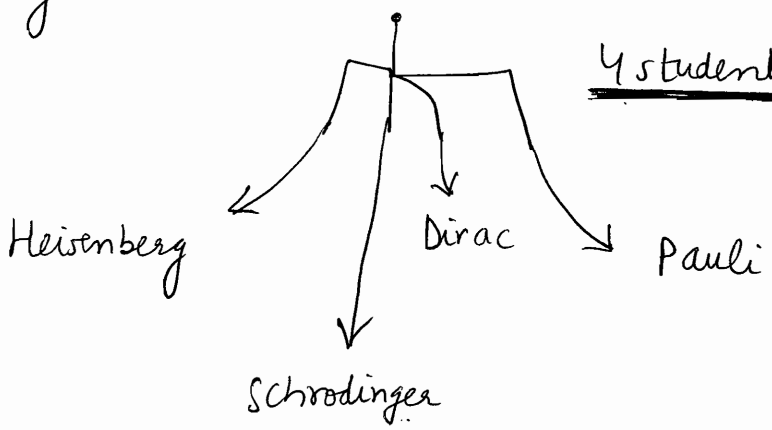
Use of this defn eliminates random constants associated with ψ due to normalization & simplifies calculations

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

<u>1926 - 1930</u>

Copenhagen : Niel's Bohr

<u>4 students</u> (25-30 years)



<u>Representation of A in Matrix Form</u> : Heisenberg's description

$A =$ Matrix Form

$= A[I]_n$

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

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

<u>Representation in Bracket Form</u> : Dirac's description

BRAKET

$$\underbrace{\langle \psi |}_{} A \underbrace{| \psi \rangle}_{} = \int \psi^* A \psi \, d\tau$$

$\langle \, |$: Bra : ψ^*

$| \, \rangle$: ket : ψ

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

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

$$\langle a \rangle = \langle \psi | A | \psi \rangle = \underset{\substack{\uparrow \\ n^{th} \text{ state}}}{\langle n} | A | n \rangle$$

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.

  $\Rightarrow$ Addition, Multiplication of Operators like Matrices

  $\Rightarrow$ $AB \neq BA$

- Eigen Value Problem

$$A \psi_n = a_n \psi_n$$

where $|\psi\rangle$ — Eigen states or Eigen Functions

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

→ These 2 are solutions of the above eqn!!

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

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

if ψ is normalized function वरना divide भी करना पड़ेगा!!

- Momentum

$$\underbrace{p_x}_{a} \psi = \underbrace{-i\hbar \frac{\partial}{\partial x}}_{A} \psi$$

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

Kinetic Energy

$$\underbrace{T}_{a} \psi = \underbrace{\frac{-\hbar^2}{2m} \frac{\partial^2}{\partial x^2}}_{A} \psi$$

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

This is 2nd order differential equation.

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

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

Solution :- $\psi_x = Ae^{ikx} + Be^{-ikx}$ [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

$$\boxed{[A, B] = AB - BA}$$ (where A & B are operators)

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

i.e. $AB = BA$

* If A and B are commutative i.e. $AB = BA$
$\Rightarrow$ 'a' and 'b' variables are simultaneously measurable

(remember corollary to Kronecker Delta Function)

* $\Rightarrow$ they are satisfied by same eigenfunction.

To measure 'a' in state ψ $\Rightarrow$ $A\psi = a\psi$ — (1)

and also measure 'b' in same state ψ $\Rightarrow$ $B\psi = b\psi$ — (2)

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

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

$$BA\psi \Rightarrow Ba\psi = aB\psi = ab\psi \quad — (1)$$

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

$$\Rightarrow AB\psi = Ab\psi = bA\psi = ab\psi \quad — (2)$$

(2) − (1)

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

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

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

★ If 2 dynamical variable's operators have same eigen function, then the 2 operators are commutative !!

eg.

$$\left[p_x, \frac{p_x^2}{2m}\right] = 0$$

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

(units : per second)

Probability Current Density

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

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

★ Operation पहले normal पे, फिर conjugate पे !!

refer Ch-11

$$\boxed{\vec{J} = \frac{\hbar}{2mi}\left[\psi^* \vec{\nabla}\psi - \psi \vec{\nabla}\psi^*\right]}$$

- It is fraction of particles (scattered or crossing or transmitted)/(incident) [redacted] per unit time.

Wave $\iff$	EM $\iff$	Quantum
Intensity	Poynting Vector	Prob. Current Density

Same thing in various subjects.....

From Continuity Condition,

$$\underset{\substack{\uparrow \\ \text{Current density}}}{\vec{\nabla}\cdot\vec{J}} + \left(\frac{\partial \rho}{\partial t}\right) = 0$$

Charge density

[valid for conservation of charge / mass]

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

[redacted] In 1-d, $\boxed{\dfrac{dJ_x}{dx} + \dfrac{d\rho}{dt} = 0}$

ρ: Probability density $= \psi^*\psi$

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

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,

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

[redacted]

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

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

(*) For hermitian Operator

$$\psi^* V\psi = \psi V^*\psi^*$$

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

(*)

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

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

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

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

$\psi = \sin nx$

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....

Q 31/ Tut 2

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

$\rho = 1$

$$= \frac{\hbar}{2mi}\, 2ik = \frac{\hbar k}{m} = \frac{p}{m} = v$$

32 $$H = -\frac{d^2}{dx^2} + x^2$$

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

Eigen Function if

$$H\psi = \lambda \psi$$ where λ can be any number

$$-\frac{d}{dx}\left[A e^{-x^2/2} - A x^2 e^{-\frac{x^2}{2}}\right] + x^2\left[A x e^{-\frac{x^2}{2}}\right]$$

$$= 3 A x e^{-\frac{x^2}{2}} = 3\psi$$ $\boxed{\text{Eign Value} = 3}$

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

(1-d case)

$$\Rightarrow \int_{-\infty}^{\infty} \psi^* \psi \, dx = 1$$

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

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

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

$$\psi(x) = \left(\frac{2}{\sqrt{\pi}}\right)^{\frac{1}{2}} e^{-2x^2}$$

Yes ; eigenvalue $= 4\alpha$

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

$$P_x = \int_{-\infty}^{0} \psi^* \psi \, dx = \frac{2}{\sqrt{\pi}} \int_{-\infty}^{0} e^{-4x^2} dx$$

Put $4x^2 = y$

$8x \, dx = dy$

$$= \frac{2}{\sqrt{\pi}} \int_0^{\infty} e^{-4x^2} dx$$ [even function]

$$= \frac{2}{\sqrt{\pi}} \cdot \frac{1}{2(4)^{\frac{1}{2}}} \Gamma\tfrac{1}{2} = \frac{2}{\sqrt{\pi}} \cdot \frac{1}{4}\sqrt{\pi} = \left(\frac{1}{2}\right)$$

(iv) Yes

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

$$\int \psi_m^* \psi_n \, d\tau = 0$$

$$\int x \, \psi^* \psi \, d\tau = 0 \qquad \int_{-\infty}^{\infty} x \, e^{-4x^2} dx = 0$$

↑
odd function
Hence LHS = 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

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

✓ 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 $\quad X(P_{max}) = 1$

$$\langle X \rangle = \left(\frac{11}{6}\right)$$

✓ All the problems defined in course are <u>time independent</u>.
i.e. <u>Stationary State Solutions</u>

eg. e^- in 1 state : time independent energy

<u>but if</u> [e^- jumps from 1^{st} to 2^{nd} state : time dependent energy
Current in superconductors : time dependent .... $\left(\frac{dq}{dt}\right)$

$H \psi_n = E_n \psi_n$: Schrodinger Wave Eqⁿ

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

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

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

the most standard form of Schrödinger Wave Equation

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

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

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

Hence this k is the familiar wave number.

We know, classically $E = T + V$.

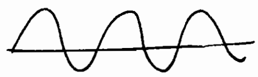
$E - V = T > 0$ (classically)

$\Rightarrow E - V > 0$

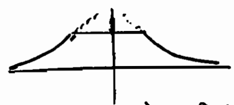
$\Rightarrow +k^2 \Rightarrow$ Trigonometric Solution

If anyhow $-k^2 \Rightarrow$ Exponential Solution

• जो हम classically



waves form करते आ रहे हैं !!



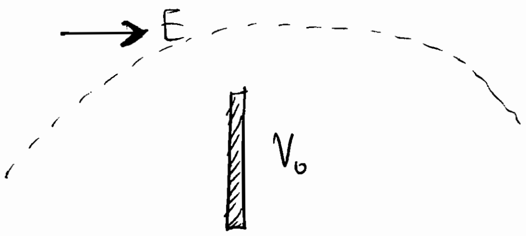
• जहाँ type के solution जो exponentially drop off कर रहे हैं

if $(E-V) > 0$

$$\Rightarrow \psi_{(x)} = \underset{\longrightarrow +x}{A e^{ikx}} + \underset{\longleftarrow -x}{B e^{-ikx}}$$

: Standing wave : Confined to a region

V_0: Potential Barrier

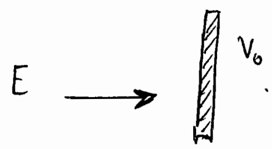


[classically]

⊙ 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

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

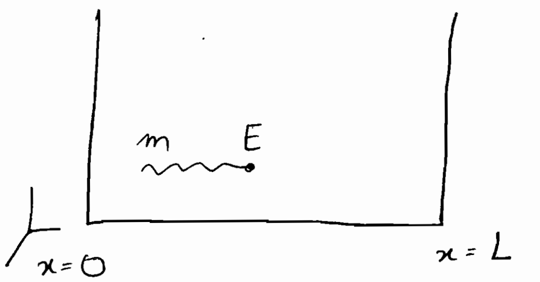
$$\frac{d^2\psi}{dx^2} - k'^2\psi = 0 \qquad k'^2 = \frac{2m}{\hbar^2}(V-E)$$

$$\psi_x = Ae^{k'x}u(x) + Be^{-k'x}u(x)$$

$-\infty < x < 0 \quad : \quad Ae^{k'x}$

$0 < x < \infty \quad : \quad Be^{-k'x}$

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



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

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

$$V = 0 \qquad H = \frac{p^2}{2m}$$

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

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

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

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

A cannot be 0, otherwise wave Function will vanish

$$\Rightarrow kL = n\pi \qquad n = 1, 2, 3, \ldots$$

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

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

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

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

- Note that solution of eigen ~~values~~ value problems are eigen functions and eigen values

$$A\psi = a\psi$$

Solution : ψ_n , a_n

Normalizing Wave Function

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

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

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

$$\Rightarrow \boxed{\begin{aligned} \psi_n(x) &= \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi x}{L}\right) \\ E_n &= n^2 \left(\frac{\pi^2 \hbar^2}{2mL^2}\right) \end{aligned}}$$

Final solutions are represented in terms of Quantum Numbers

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

(1) What we assumed that different "loops of stationary waves" or "eigen functions" are nothing but different "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 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)

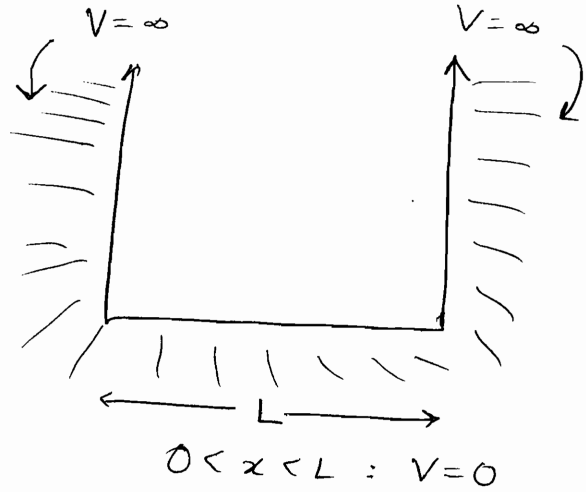
10/02/2012

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

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

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



- Boundary Conditions due to ∞ potential

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

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

Solution gives :

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

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

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

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

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

Commensurate with de Broglie's wave : ✓

Commensurate with Heisenberg Principle :

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

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

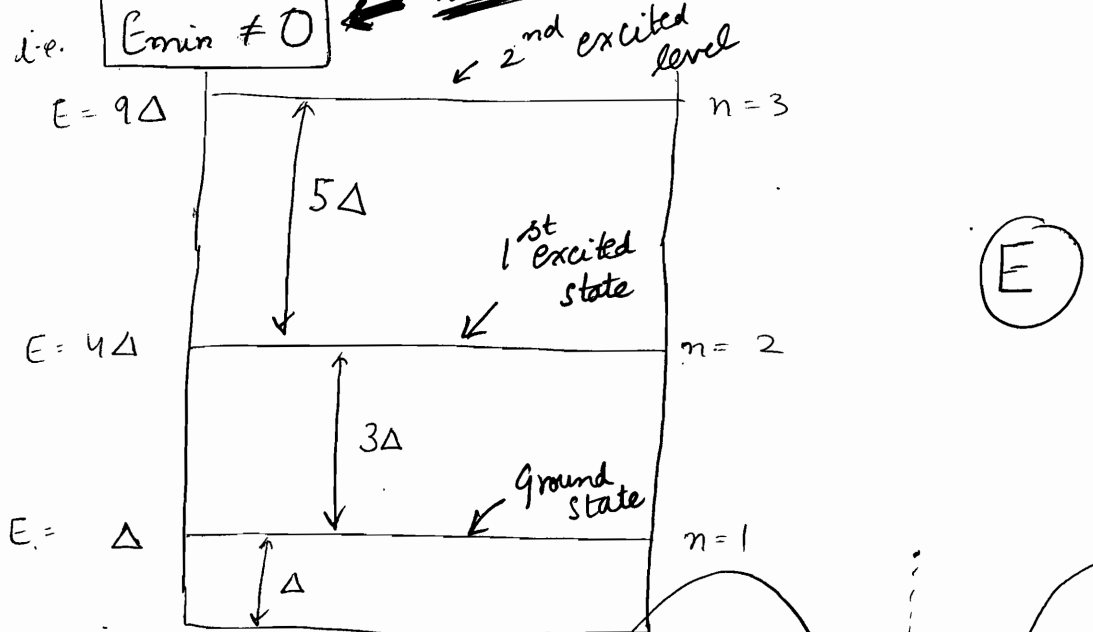
$$\Delta p_x \geq \frac{\hbar}{2L}$$

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

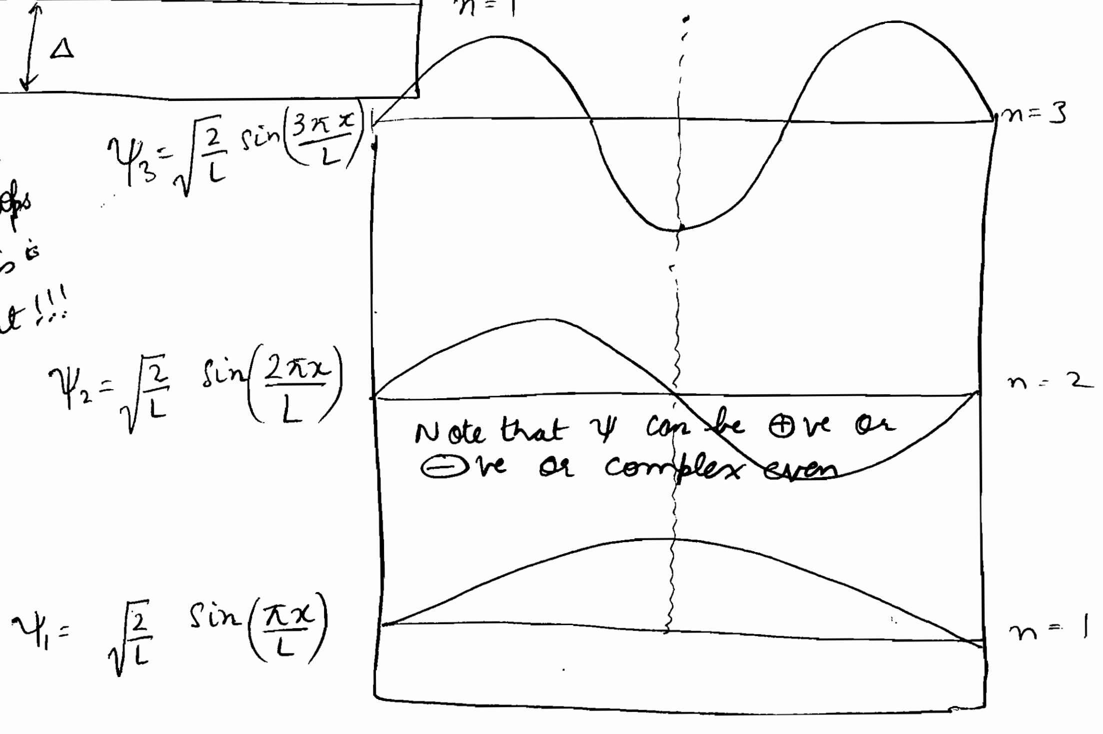
$$E \geq \frac{\hbar^2}{4L^2 . 2m} = \frac{\hbar^2}{8mL^2} \qquad E_{min} = \frac{\hbar^2}{8mL^2}$$

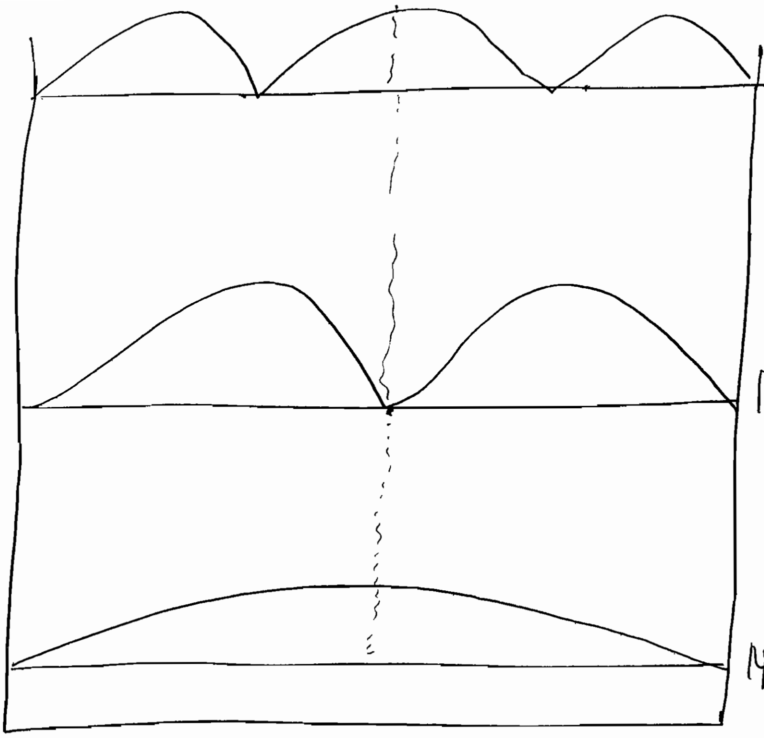
Told by Quantum Mechanics !!

i.e. $\boxed{E_{min} \neq 0}$



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





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

$\boxed{|\psi|^2}$

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

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

n^{th} state $\Rightarrow$ n maximas 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,

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

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

$\Rightarrow$ either $\sin\left(\frac{2\pi x}{L}\right) = 0 \Rightarrow x = \frac{n\pi L}{2\pi} = \left(\frac{nL}{2}\right)$

or

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

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

Q/ What is meant by $\langle\psi^* x\, \psi\rangle$??

↑ Expectation value

dice $\{1,1,6,1,1,1\}$

P_x max @ $x=1$

$\langle x\rangle = \frac{5}{6}\cdot 1 + \frac{1}{6}\cdot 6 = \left(\frac{11}{6}\right)$

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.

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

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

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

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

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

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

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

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

Note this term also $\longrightarrow$ $-\frac{L^2}{8\pi^2}$

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

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

$$= 0$$

$\boxed{\langle p_x \rangle = 0}$ Almost Always ... (when ψ is real)

$\langle p_x^2 \rangle \neq 0$ otherwise $T = 0$ which is never the case.

$$\langle p_x^2 \rangle = \langle \psi \mid P_x^2 \mid \psi \rangle$$

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

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

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

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

$$= \cancel{\left(\frac{h^2 n^2}{4L^2}\right)} \quad \left(\frac{\hbar^2 n^2 \pi^2}{L^2}\right)$$

$$\Rightarrow \Delta p_x = \cancel{\left(\frac{nh}{2L}\right)} \quad \left(\frac{n\pi\hbar}{L}\right)$$ ✓

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

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

$$\Delta p_x \Delta x = \frac{n\pi\hbar}{L} \cdot \frac{L}{\sqrt{12}} \geq \frac{\pi\hbar}{\sqrt{12}} = \left(\frac{\hbar}{1.1}\right) > \left(\frac{\hbar}{2}\right)$$

Easy way

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

as it is eigenstate of Hamiltonian

But for free particle

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

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

$$\Delta p = \sqrt{\langle p^2 \rangle - \langle p \rangle^2} = \left(\frac{nh}{2L}\right)$$

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

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

Q| If $\psi_x = \frac{1}{\sqrt{14}}\phi_1(x) + \frac{9}{\sqrt{14}}\phi_2(x) + \frac{3}{\sqrt{14}}\phi_3(x)$

and Particle is trapped in 1-d box.

Find $\langle E\rangle$.

$\boxed{\text{Refer Q1 - P 152 of Verma}}$

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 $|\psi_{(x)}\rangle = c_1\phi_1 + c_2\phi_2 + c_3\phi_3$

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

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

$$\underbrace{c_1^*c_1\langle\phi_1|\phi_1\rangle}_{=c_1^*c_1 = |c_1|^2} + \underbrace{c_1^*c_2\langle\phi_1|\phi_2\rangle}_{=0} + \underbrace{c_1^*c_3\langle\phi_1|\phi_3\rangle}_{=0}$$

(Kronecker δ function)

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

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

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

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

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

$$\langle E \rangle = \langle \psi | H | \psi \rangle / \langle \psi | \psi \rangle$$

$$= \frac{1}{14} \langle \phi_1 | H | \phi_1 \rangle + \frac{4}{14} \langle \phi_2 | H | \phi_2 \rangle + \frac{9}{14} \langle \phi_3 | H | \phi_3 \rangle$$

★ Note that for deep well wave functions $\phi_1, \phi_2, \ldots$

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

but

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

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

[We know $\langle \psi_n | H | \psi_n \rangle = \dfrac{n^2 h^2}{8mL^2}$]

$$\langle E \rangle = \frac{1}{14} \cdot \left(\frac{h^2}{8mL^2}\right) + \frac{4}{14} \cdot 4 \left(\frac{h^2}{8mL^2}\right) + \frac{9}{14} \cdot 9 \left(\frac{h^2}{8mL^2}\right)$$

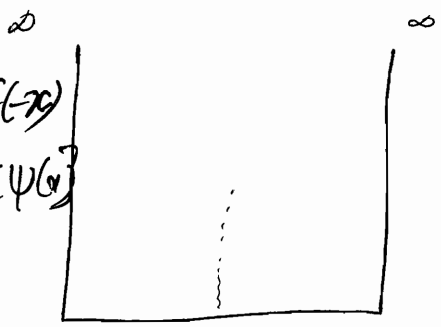
$$= \frac{1+16+81}{14} \cdot \frac{h^2}{8mL^2} = \frac{\cancel{98}^{\,7}}{\cancel{14}_{\,2} * 8} \cdot \frac{h^2}{mL^2}$$

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

Infinite Energy Well Problem with changed coordinates

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

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



$\Pi [f(x)] = f(-x)$

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

→ common eigenfunctions

→ energy eigenfunction = odd or even

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

Writing the eqn,

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

$$\Rightarrow \underline{\psi_1 = A \sin kx + B \cos kx}$$

Hamiltonian → with Parity commutes Function if V is even

Boundary Conditions

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

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

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

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

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

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

From (1)

either $B = 0 \quad \Rightarrow \quad \psi_1 = A \sin(kx)$

or

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

From (2)

either $A = 0 \quad \Rightarrow \quad \psi_1 = B \cos kx$

or

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

$\boxed{\text{Closed Form Solutions}}$ $\Rightarrow$ Both $A \sin kx$ and $B \cos kx$ are solutions.

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

$\cancel{\psi_1 = A \sin kx}$

$$\psi\left(x = \pm\frac{a}{2}\right) = 0 \quad \Rightarrow \quad k\frac{a}{2} = n\pi \quad \Rightarrow \quad k = \left(\frac{2n\pi}{a}\right)$$

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

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

$\psi_2 = B\ \cancel{\cos kx}$

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

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

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

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

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

This way we should write down final equation!!

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

Final solution are represented in terms of Quantum Numbers.....

We can combine the 2 solutions as

$$\psi_n = \sqrt{\frac{2}{a}}\left[\sin\left(\frac{2n\pi x}{a}\right) + \cos\frac{(2n-1)\pi x}{a}\right]$$

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]

Q1) $\psi(q,t) = \psi(q,0)\, e^{-i\omega t} = A e^{-i\omega t}$

Expansion Coefficient

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

$$\left[\text{Fourier} \quad f(x) = \frac{1}{\sqrt{2\pi}} \int F(k)\, e^{ikx}\, dk \right]$$ Not required

Normalization

$$\int_0^a \psi^* \psi \, dq = |A|^2 a = 1$$

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

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

$$F(k) = \frac{1}{\sqrt{2\pi}} \int_0^a \frac{1}{\sqrt{a}} e^{-i(\omega t + kx)}\, dx$$

$$= \frac{1}{\sqrt{2\pi a}} \left[\frac{e^{-i(\omega t+kx)}}{-ik} \right]_0^a$$

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

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

$$= \frac{1}{\sqrt{2\pi a}} \frac{e^{-ika} - 1}{-ik}$$

Q29)

$$H\psi = E\psi$$

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

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

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

Q30)

$$\boxed{\begin{array}{ll} 3^{rd} \text{ excited} : & n = 4 \\ \text{ground} : & n = 1 \end{array}}$$ ★ ★ This was taught by P. Bahadur

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

$$\Rightarrow 60\,eV = \frac{15h^2}{8mL^2}$$

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

$$= 0.094 \times 10^{-18}$$

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

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

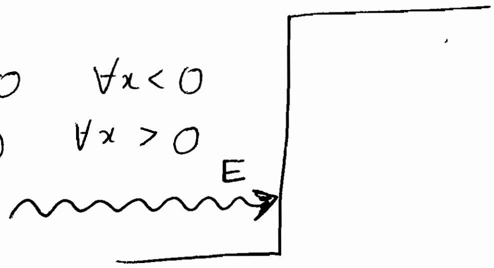
Quantum Physics (6)

11/02/12

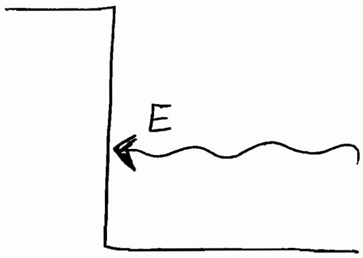
Problem of Step Potential

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

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



(Ascending step potential)



(descending step potential)

⊙ We need to work out

$$\boxed{T = \left(\frac{J_T}{J_I}\right) = \left(\frac{\text{Transmitted Flux}}{\text{Incident Flux}}\right)} \qquad \boxed{R = \left(\frac{J_R}{J_I}\right) = \frac{\text{Reflected Flux}}{\text{Incident Flux}}}$$

Transmittance = fraction of particle transmitted

Reflectance = fraction of particles reflected

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

Hence to calculate coefficients we need to find out functions ψ_I, ψ_R, ψ_T

We have Schrodinger Wave Equation at our disposal.

For $x < 0$ $\quad H\psi_1 = E\psi_1$

$$\Rightarrow \frac{d^2\psi_1}{dx^2} + \frac{2m(E-V)\psi_1}{\hbar^2} = 0$$

$$\Rightarrow \frac{d^2\psi}{dx^2} + \frac{2m}{\hbar^2}E\psi_1 = 0$$

$$\Rightarrow \psi_1 = A e^{ik_1 x} + B e^{-ik_1 x} \qquad k_1^2 = \frac{2mE}{\hbar^2}$$

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

$\boxed{E > V_0}$ Classically Feasible Case....
Quantum Mechanically non important case....

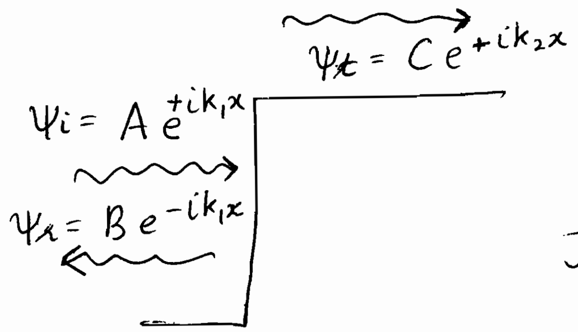
$$\frac{d^2\psi_2}{dx^2} + \frac{2m}{\hbar^2}(E - V_0)\psi_2 = 0$$

$$\Rightarrow \frac{d^2\psi_2}{dx^2} + k_2^2\psi_2 = 0 \qquad \text{where } k_2^2 = \frac{2m}{\hbar^2}(E - V_0)$$

$$\psi_2 = \underline{C e^{ik_2 x}} + D e^{-ik_2 x}$$

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

$$\Rightarrow \psi_2 = C e^{ik_2 x}$$



$J = \rho v$
$= |\psi|^2 \cdot \frac{p}{m}$
$= \frac{|\psi|^2 k\hbar}{m}$ (for exp)

$\boxed{\text{Step 1}}$ Calculating J

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

$$= \frac{\hbar}{2mi} 2AA^* k i = \frac{\hbar k_1 AA^*}{m} = \frac{\hbar k_1 |A|^2}{m}$$

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

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

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

Reflectance or

$$\frac{R: \text{fraction of particles reflected}}{T: \text{fraction of particles transmitted}}$$

or

Transmittance

$$\Rightarrow \boxed{R = \frac{BB^*}{AA^*}} \qquad \boxed{T = \frac{k_2\, CC^*}{k_1\, AA^*}}$$

Step II Applying Boundary Conditions

(Single valued Function)

$$\psi_1 = \psi_2$$

$$\Rightarrow A + B = C \quad \text{--- (1)}$$

(continuous at $x=0$)

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

$$\Rightarrow ik_1(A-B) = ik_2 C \quad \text{--- (2)}$$

From (1) and (2),

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

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

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

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

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

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

Fraction of flux reflected ✓

Fraction of flux transmitted ✓

Q1)

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

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

Q11)

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

$E - V_0 = 1$

$E = 1.5$

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

$$T = 1 - R$$

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

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

CASE 2 $E < V_0$

Classically Forbidden Case
Quantum Mechanically Important Case

Region 1

$$\psi = \underline{A e^{ik_1 x}} + \underline{B e^{-ik_1 x}} \qquad k_1 = \sqrt{\frac{2mE}{\hbar}}$$

Region 2

Step I

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

$$\Rightarrow \frac{d^2\psi_2}{dx^2} - k_2^2 \psi_2 = 0 \qquad k_2 = \sqrt{\frac{2m(V_0-E)}{\hbar^2}}$$

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 $x \to \infty$, $\psi_2 \to 0$)

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

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

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

$$J_t = 0$$

Step II : Boundary Conditions

Single valued : $A + B = C$

Continuity $\left.\frac{d\psi_1}{dx}\right|_{x=0} = \left.\frac{d\psi_2}{dx}\right|_{x=0} \Rightarrow A - B = -\frac{k_2 C}{k_1 i} = \frac{i k_2 C}{k_1}$

Adding $A = \left(1 + \frac{ik_2}{k_1}\right)\frac{C}{2}$

Subtracting $B = \left(1 - \frac{ik_2}{k_1}\right)\frac{C}{2}$

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

$$\underline{T = \frac{J_T}{J_i} = 0}$$

But $\boxed{|C|^2 \neq 0}$

$$J_t = \frac{\hbar}{2mi} \left[\psi_t^* \frac{\partial \psi_t}{\partial x} - \psi_t \frac{\partial \psi_t^*}{\partial x} \right] \qquad \psi_t = Ce^{-k_2 x}$$

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

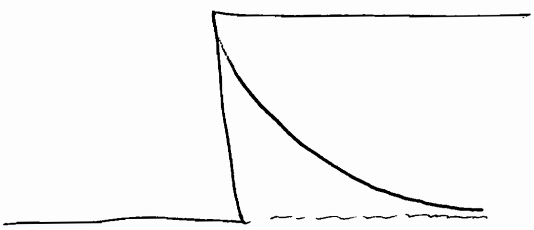
$$= 0$$

$\Rightarrow T$ should be 0

→ This is what we expected Classically

but $C \neq 0$

ie. there is some probability of particle being in Region 2.



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

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

$\underline{Prob = P_{max} \, e^{-2k_2 x}}$

ie. <u>even when no particle is crossing, there is some probability of particle being present there.</u>

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

$$\psi_d = \frac{1}{e}\psi_{max}$$

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

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

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 $\psi = Ce^{-}$ we get $\boxed{\Delta x = \frac{1}{2k_2}}$

$$p_x = \hbar k_2$$

$$\Delta p_x = \hbar k_2$$

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

if $E = E + \Delta E$

$\Rightarrow \Delta E = V_0 - E$

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

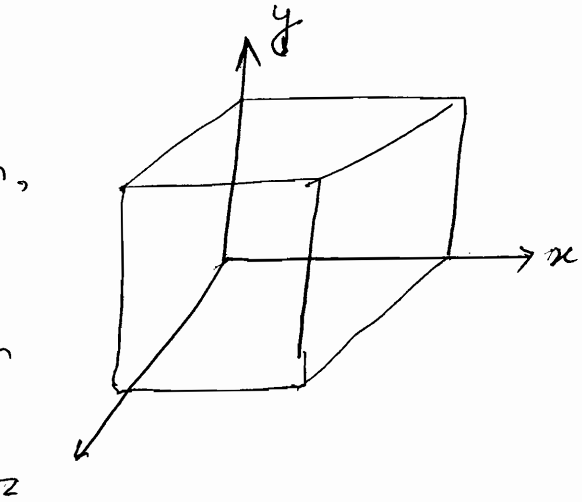
$$\Delta p_x = \sqrt{2m(V_0-E)}$$

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

★ या तो $\left(\frac{1}{\gamma}\right)$ ले लो
या तो $\Delta E = (V_0-E)$ ले लो!!

Particle in a 3-d box or Cubical Box

- Length of side = L
- Particle of mass m, trapped in 3-d Box.



Free to move between

x : 0 to L
y : 0 to L
z : 0 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.

$$\Rightarrow \quad E = T$$

Using Schrodinger Wave Equation,

$$H\psi = E\psi$$

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

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

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

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

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

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

In 3 dimension, (Writing k as a composition of 3-dimensional k-space)

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

Such Partial derivative equation is always worked out by Separation of Variables

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

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

$\Rightarrow$ 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.

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

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

at $x = L$,

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

$$\Rightarrow \boxed{k_x = \frac{n_x \pi}{L_x}} \quad \boxed{k_y = \frac{n_y \pi}{L_y}} \quad \boxed{k_z = \frac{n_z \pi}{L_z}}$$

$$\Rightarrow \boxed{X(x) = \sqrt{\frac{2}{L_x}} \sin\left(\frac{n_x \pi x}{L_x}\right)} \qquad n_x = 1, 2, 3, \ldots\ldots$$

Similarly,

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

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

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

Also $\boxed{k_x^2 + k_y^2 + k_z^2 = k_R^2 = \frac{2mE}{\hbar^2}}$

⊙ 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

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

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

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

For cubical box,

$$\Delta' = \frac{h^2}{8mL^2}$$

eigen values $\rightarrow$
$$\boxed{E_{(n_x, n_y, n_z)} = \frac{\hbar^2 \pi^2}{2mL^2}\left[n_x^2 + n_y^2 + n_z^2\right]}$$

eigen funct. $\rightarrow$
$$\boxed{\psi(x,y,z) = \sqrt{\frac{8}{L^3}} \sin\left(\frac{n_x \pi x}{L}\right) \sin\left(\frac{n_y \pi y}{L}\right) \sin\left(\frac{n_z \pi z}{L}\right)}$$

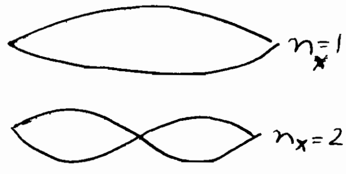
Any of the 3 quantum numbers, $n_x, n_y, n_z \neq 0$

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.

$\Rightarrow$ **n Corresponds to number of loops !!!** (as in 1-d case)



g_i : space degeneracy

$$H\psi = E\psi$$

$$H\psi_{(1,1,1)} = 3\Delta\, \psi_{(1,1,1)}$$

3 degenerate states i.e. same eigen value but different states
$$\begin{cases} H\psi_{(2,1,1)} = 6\Delta\, \psi_{(2,1,1)} \\ H\psi_{(1,2,1)} = 6\Delta\, \psi_{(1,2,1)} \\ H\psi_{(1,1,2)} = 6\Delta\, \psi_{(1,1,2)} \end{cases}$$

- $E = 14\Delta$: $\psi(1,2,3)$ $\quad g_6 = 6$
- $E = 12\Delta$: $\psi(2,2,2)$ $\quad g_5 = 1$
- $E = 11\Delta$: $\psi(3,1,1)$ or $\psi(1,3,1)$ or $\psi(1,1,3)$ $\quad g_4 = 3$
- $E\ 9\Delta$: $\psi(2,2,1)$ or $\psi(2,1,2)$ or $\psi(1,2,2)$ $\quad g_3 = 3$
- $E = 6\Delta$: $\psi(2,1,1)$ or $\psi(1,2,1)$ or $\psi(1,1,2)$ $\quad g_2 = 3$
- $E = 3\Delta$: $\psi_{(1,1,1)} = \sqrt{\frac{8}{L^3}} \sin\left(\frac{\pi x}{L}\right) \sin\left(\frac{\pi y}{L}\right) \sin\left(\frac{\pi z}{L}\right)$ $\quad g_1 = 1$

$g_1 = 1$: 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

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

example: ✓ I have to fill $10e^-$ without taking spin into account.

Energy (no. of e^-)

[redacted]

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

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

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

Tut3 Q 15

Density of States

We know,

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

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

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

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

↑

Sphere of radius R

$\boxed{\text{density of states}}$

↳ $\boxed{g = \frac{dN}{dE}}$

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

$n_x, n_y, n_z \longrightarrow E$

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

⊛ do not get confused

Previous 'g' was degeneracy

This 'g' is density of state

$\boxed{\text{refer P-311}}$

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

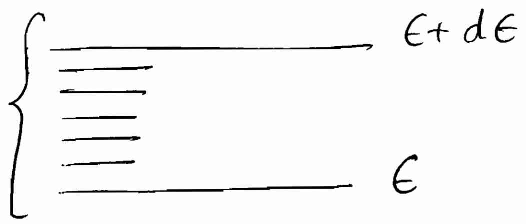
We need to find dN where k changes from k to k+dk

where Energy is related to states as

N = no. of states

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

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



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

dN = No. of energy states between E and E+dE are energy states lying between radius : R and R+dR

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

[Note that Quantum Numbers are POSITIVE] ⇒ only 1 octant

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

$$= \frac{1}{8} \underbrace{\left[\frac{4\pi}{3} (R + dR)^3 - \frac{4\pi}{3} R^3 \right]}$$

$$= \frac{4\pi R^3}{3}\left[1 + 3\frac{dR}{R}\right] - \frac{4}{3}\pi R^3$$

$$= \frac{1}{8} \cdot 4\pi R^2 dR$$

$$= 4\pi R^2 dR$$

Now we know,

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

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

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

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

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

- अरे भयया !! $g(\epsilon)$ को ही तो density of state बोलते हैं !!

$$\boxed{dN = g(\epsilon) \, d\epsilon}$$

$$\Rightarrow \boxed{g(\epsilon) = \frac{2\pi V}{\hbar^3} (2m)^{\frac{3}{2}} E^{\frac{1}{2}}} \Leftarrow \text{density of states}$$

★ 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.

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 $\left(\frac{\pi}{L}\right) * \left(\frac{\pi}{L}\right) * \left(\frac{\pi}{L}\right) = \left(\frac{\pi^3}{L^3}\right)$ volume

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

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

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

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

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

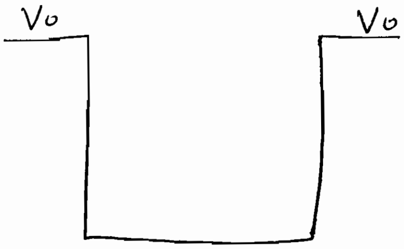
$$\Rightarrow \boxed{\left(\frac{dN}{dE}\right) = 2\pi V \frac{(2m)^{3/2}}{\hbar^3} \sqrt{E}}$$

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



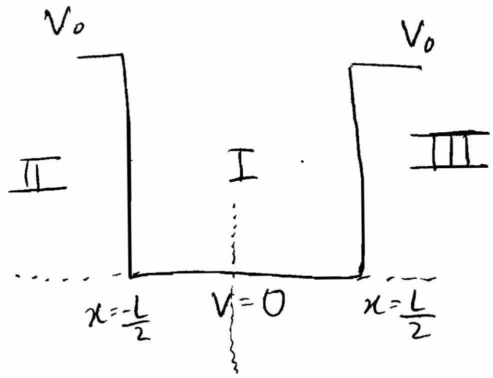
if V_0 is finite $\Rightarrow$ Finite (Potential) Well Problem (on both sides)

or

Step Potential Problem (on 1 side)

if $V_0 \to \infty$ $\Rightarrow$ Infinite (Potential Well) Problem.

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



as

$$\boxed{\begin{aligned} |x| < \frac{L}{2}, \quad V = 0 \\ |x| > \frac{L}{2}, \quad V = V_0 \end{aligned}}$$

now we will solve for this

or

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

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

- Since reference axis in between, we will get closed form of solutions.

We can solve corresponding solutions....

Step I

For I :

$$\frac{d^2\psi_1}{dx^2} + \frac{2m}{\hbar^2}(E)\,\psi_1 = 0 \qquad (V=0)$$

$$\boxed{\psi_1 = A\cos k_1 x + B\sin k_1 x} \Leftarrow \text{closed form solutions}$$

For II

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

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

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

$\longleftarrow$

For III

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

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

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

$\longrightarrow$

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

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

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

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

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

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

Step II Applying Boundary Conditions, we get complete solution

$$\underline{\psi_1 = A \sin k_1 x} \qquad\qquad \underline{\psi_1 = B \cos k_1 x}$$

$$\psi_2 = C e^{k_2 x} \qquad\qquad \psi_2 = C e^{k_2 x}$$

$$\psi_3 = D e^{-k_2 x} \qquad\qquad \psi_3 = D e^{-k_2 x}$$

Assymmetric solution

Symmetric Solution

[Sine is antisymmetric] while [cosine is symmetric]

2 possible solutions

Taking Assymmetric Solution 1st,

$\psi_1 = \psi_2$

$\frac{d\psi_1}{dx} = \frac{d\psi_2}{dx}$

$$-A \sin k_1 \frac{L}{2} = C e^{-k_2 \frac{L}{2}}$$

$$k_1 A \cos k_1 \frac{L}{2} = k_2 C e^{-k_2 \frac{L}{2}}$$

$$\Rightarrow \boxed{-k_1 \cot\left(\frac{k_1 L}{2}\right) = k_2}$$

- किसी भी एक side पर दोनों conditions ले लो !!

$\psi_1 = \psi_3$

$\frac{d\psi_1}{dx} = \frac{d\psi_3}{dx}$

$$A \sin k_1 \frac{L}{2} = D e^{-k_2 \frac{L}{2}}$$

$$k_1 A \cos \frac{k_1 L}{2} = -k_2 D e^{-k_2 \frac{L}{2}}$$

$$\Rightarrow \boxed{-k_1 \cot\left(\frac{k_1 L}{2}\right) = k_2}$$

..... redundant Boundary Condition

If we take Symmetric Solution, we get

$$\boxed{+k_1 \tan\left(\frac{k_1 L}{2}\right) = k_2}$$

Step 3

$$\boxed{x > 0 \text{ and } y > 0}$$

Multiply Symmetric Solution by $\left(\frac{L}{2}\right)$

$$\underbrace{k_1 \frac{L}{2}}_{x} \tan k_1 \frac{L}{2} = \underbrace{k_2 \frac{L}{2}}_{y}$$

$$x \tan x = y$$

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

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

Assymmetric Solution

$$\boxed{\tan(90 + \theta) = -\cot\theta}$$

$$-x \cot x = y$$

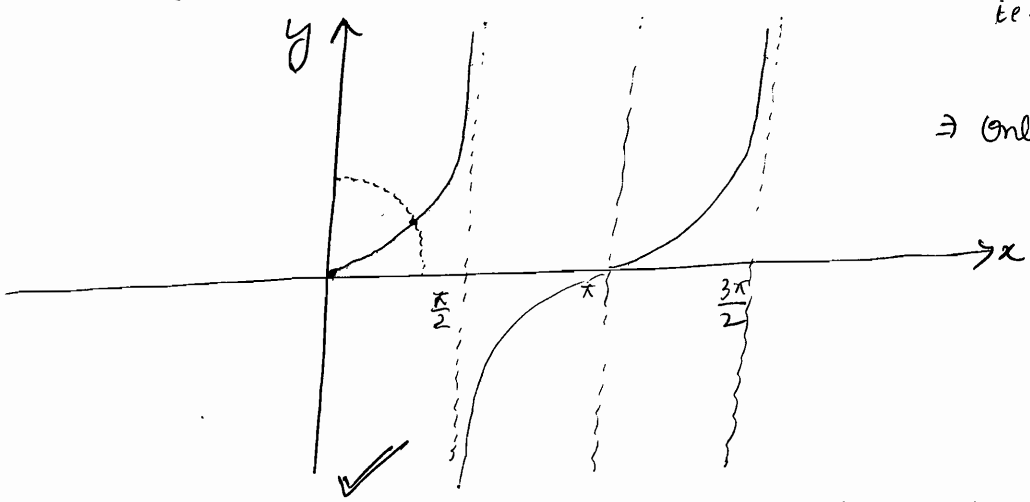
$$x \tan\left(\frac{\pi}{2} + x\right) = y$$

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.

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

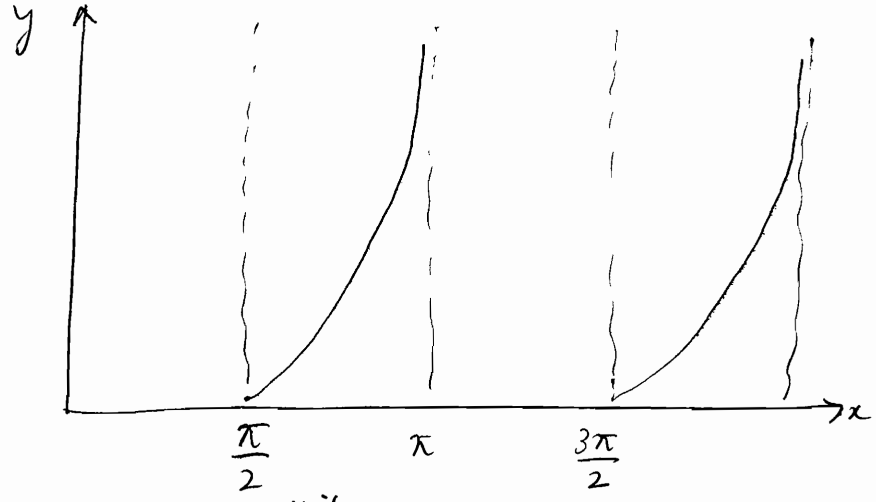


if $R < \frac{\pi}{2}$

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



$y = x \cot x$

Ground state is always symmetric solution है होता !!

If $R < \frac{\pi}{2}$, no assymmetric solution

R	Possible Symmetric Solutions	Possible Assymmetric or Anti-symmetric Solutions
$< \frac{\pi}{2}$	1	0
$= \frac{\pi}{2}$	1	1
$\frac{\pi}{2} \leq R < \pi$	1	1
$\pi \leq R < \frac{3\pi}{2}$	2	1

We will write as $\pi^2 < R^2 < \frac{9\pi^2}{4}$

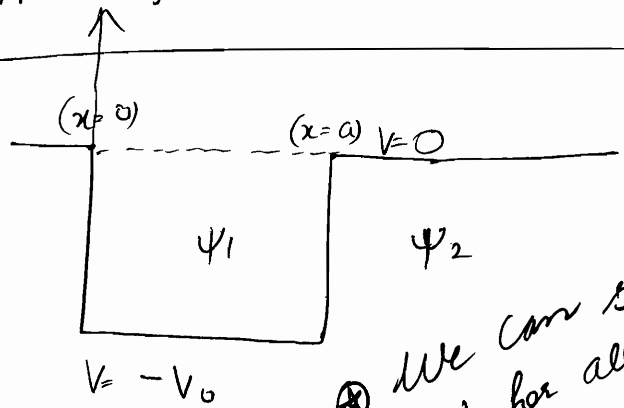
i.e. for, $\frac{2\pi^2\hbar^2}{m} < V_0 L^2 < \frac{18\pi^2\hbar^2}{m}$

we have 3 possible states.

2 symmetric and 1 anti-symmetric

Finite Well Problem has many applications.
Nucleus Attractive Well is finite.
Particle inside is trapped eg. Deutron.

Q18 / sheet



(I) $\underline{0<x<a}$

$$\frac{d^2\psi_1}{dx^2}+\frac{2m}{\hbar^2}(E-V)\psi=0$$

$$\Rightarrow \frac{d^2\psi_1}{dx^2}+\frac{2m}{\hbar^2}(-|E|+V_0)\psi_1=0$$

⊛ We can safely use $|E|$ for all calculation as there are no derivatives etc. as $|E|$ = const....

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

As $x\to 0$
$\psi\to 0$

$$\psi_1 = B = 0$$

$$\Rightarrow \boxed{\psi_1 = A\sin k_1 x}$$

(II) $\underline{x>a}$

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

$$\boxed{\psi_2 = Ce^{-k_2 x}}$$

At $x=a$,

$$A\sin k_1 a = Ce^{-k_2 a}$$

$$k_1 A\cos k_1 a = -k_2 Ce^{-k_2 a}$$

$$\Rightarrow k_1 a\cot k_1 a = -k_2 a \quad \left(\begin{matrix}\text{Multiply}\\ \text{by}\\ a\end{matrix}\right)$$

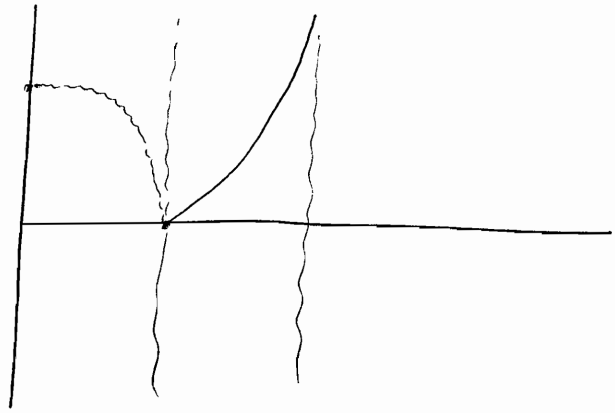
$$k_1 = \sqrt{\frac{(V_0-|E|)2m}{\hbar^2}}$$

$$\Rightarrow \boxed{x\cot x = -y}$$

$$k_2 = \frac{\sqrt{2m|E|}}{\hbar}$$

$$x^2+y^2 = \frac{2mV_0}{\hbar^2}a^2 = R^2$$

Solve.....



$$k \geq \frac{\pi}{2}$$

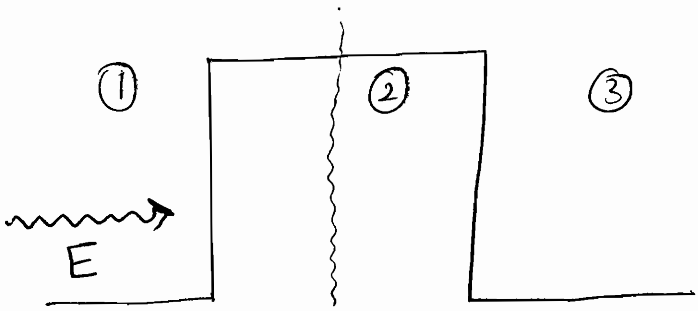
$$k^2 \geq \frac{\pi^2}{4}$$

$$\frac{2m}{\hbar^2} \cdot V_0 a^2 \geq \frac{\pi^2}{4}$$

$$\Rightarrow \quad V_0 a^2 \geq \left(\frac{\hbar^2 \pi^2}{8m}\right)$$

RECTANGULAR BARRIER

- Opposite of Finite well or 2 - step Potential Problem
- Barrier is always of finite height.



$x < \frac{-L}{2}$, $V = 0$

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

$-\frac{L}{2} < x < \frac{L}{2}$: $V = V_0$

$$R = \left(\frac{J_r}{J_i}\right) \qquad T = \left(\frac{J_t}{J_i}\right)$$

Step I : Setting of Schrodinger Equations

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

$$\psi_1 = \underline{Ae^{ik_1x}} + \underline{Be^{-ik_1x}}$$

$$R = \frac{|B|^2}{|A|^2}$$ As we did for finite step potential

(3) $$\frac{d^2\psi_3}{dx^2} + \frac{2mE}{\hbar^2}\psi_3 = 0$$

$$\psi_3 = \underline{Fe^{ik_1x}}$$ [Note that no returning wave]

$$T = \frac{|F|^2}{|A|^2}$$

(2) Quantum Mechanically, important case is $\underline{E < V_0}$

Particle crossing, if $E < V_0$, solution is called Tunneling Phenomenon.

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

$$\psi_2 = Ce^{ik_2x} + De^{-ik_2x}$$

For $E < V_0$

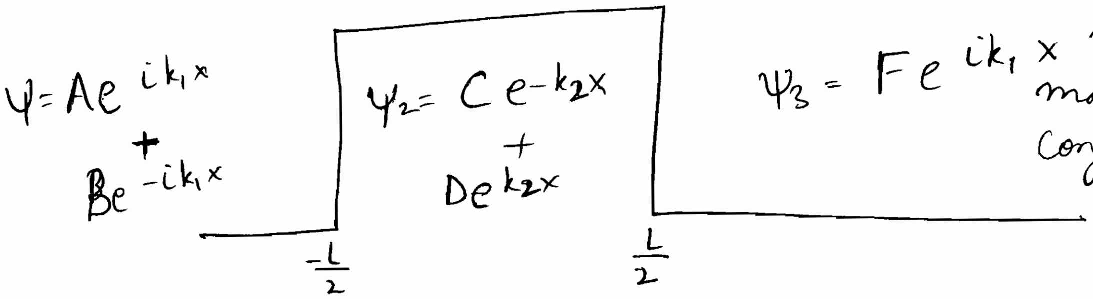
$$\frac{d^2\psi_2}{dx^2} - \frac{2m}{\hbar^2}(V_0 - E)\,\psi_2 = 0$$

$$\Rightarrow \quad \psi_2 = \underline{Ce^{-k_2 x}} + \underline{De^{k_2 x}}$$

[Note that nothing is 0 as x is finite)

Step II Boundary Conditions

✪ do not use alphabets like 'E' or 'H' or 'J' etc. for naming. They may lead to confusion.



Solve for $\left(\frac{B}{A}\right)$ & $\left(\frac{F}{A}\right)$

$\psi_1 = \psi_2$ | $Ae^{ik_1\frac{L}{2}} + Be^{-ik_1\frac{L}{2}} = Ce^{-k_1\frac{L}{2}} + De^{k_1\frac{L}{2}}$

$\frac{d\psi_1}{dx} = \frac{d\psi_2}{dx}$ | $k_1 A e^{ik_1\frac{L}{2}} - k_1 B e^{-ik_1\frac{L}{2}} = -Ck_1 e^{-k_1\frac{L}{2}} + k_1 D e^{k_1\frac{L}{2}}$

$\psi_2 = \psi_3$ | ———

$\frac{d\psi_2}{dx} = \frac{d\psi_3}{dx}$ | ———

By solving 4 equations in terms of A, we get,

(very rigorous algebra)

$$\approx \frac{16\, V_0^2}{E(V_0-E)}\left[\frac{e^{2x}+e^{-2x}}{4}+\frac{1}{2}\right]$$

neglect

$$\frac{1}{T} = 1 + \frac{V_0^2}{4E(V_0-E)}\,\underbrace{\sinh^2(k_2 L)}$$

x is large

Neglecting (1), $\frac{1}{T} = \frac{V_0^2}{4E(V_0-E)}\left(\frac{e^{2x}}{4}\right)$

$$\Rightarrow \frac{1}{T} \approx \frac{V_0^2}{4E(V_0-E)}\,\frac{e^{2x}}{4}$$

$$\Rightarrow \frac{1}{T} = \frac{V_0^2\, e^{2x}}{16\,E(V_0-E)} =$$

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)

$r_{nucleus} = 10^{-15}$ m

$m_\alpha = 4 \times 1.66 \times 10^{-27}$ kg

This problem is called <u>Quantum Mechanical Tunneling</u>.

$$\frac{16 \cdot 8 \cdot 27}{(35)^2}\, e^{-2 * \sqrt{\frac{2m\, 27}{\hbar^2}} * 10^{-15}}$$

=

Matter of fact is that α particle makes 10^{40} attempts and comes out of nucleus ... observed fact.

$$p = k\hbar$$
$$= \sqrt{2m(V_0 - E)}$$

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

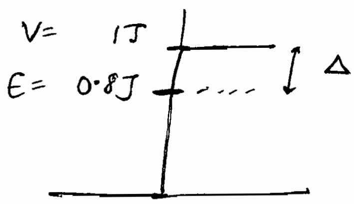
$$\Delta x = \frac{\hbar}{2\sqrt{2m(V_0 - E)}}$$

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

$$\Rightarrow V_0 = E + \Delta E$$

$$T = E - V_0 = -\Delta E$$

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

If $\Delta = -(V_0 - E)$
$\Rightarrow$ E is just equal to V
Hence, Particle can escape.

(*) Note that in Energy Uncertainty Principle, there is no inequality but rather $\Delta E \, \Delta t \approx \hbar$

(*) $\boxed{V_0 > E}$ $T = \dfrac{4E(V_0 - E)}{4E(V_0 - E) + V_0^2 \sinh^2(\gamma L)} \approx e^{-2\gamma L}$

$\boxed{V_0 < E}$ $T = \dfrac{4E(E - V_0)}{4E(E - V_0) + V_0^2 \sin^2(\gamma L)} \approx e^{-2\gamma L}$

$\boxed{R = 1 - T}$

Approximation if $\gamma L > 5$

(*) 4 examples of tunneling $\longrightarrow$
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.

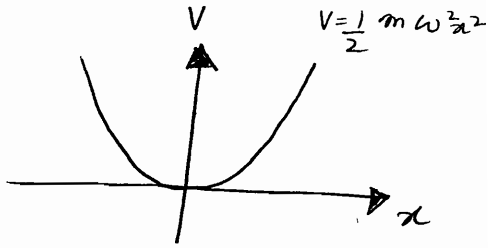
$F \propto -x$

$F = -kx$

$V = -\int F \cdot dx = \frac{1}{2}kx^2 = \frac{1}{2}m\omega^2 x^2$

$$E = \frac{p^2}{2m} + \frac{1}{2}m\omega^2 x^2$$

(T) (V)



Parabolic Potential Well

Classically, it can have any value of energy including 0.

[as $A \to 0$, $\frac{1}{2}kA^2 \to 0$]

But we need to measure Energy Quantum Mechanically.

i.e. $H\psi = E\psi$

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

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

$$\Rightarrow \boxed{\frac{d^2\psi}{dx^2} + \left[\frac{2m}{\hbar^2}(E) - \frac{m^2\omega^2 x^2}{\hbar^2}\right](\psi) = 0} \quad \text{—— (1)}$$

Note that till now, V was const., hence easy differential equations.
Now the solution of differential equation has become complex.

Step 1 Let $y^2 = \left(\frac{\sqrt{km}}{\hbar}\right)^{\frac{1}{2}} x$

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

$k = \omega^2 m$

$km = \omega^2 m^2$

$\sqrt{k} = \omega m$

i.e. $\boxed{y = \sqrt{\left(\frac{m\omega}{\hbar}\right)}\, x}$

$\boxed{y : \text{dimensionless quantity}}$

$y = \left(\frac{x}{A}\right)$ where A: Amplitude $= \sqrt{\frac{\hbar}{m\omega}}$

<u>y is a pure number</u>

$$\Rightarrow \frac{d}{dx} = \frac{d}{dy} \cdot \frac{dy}{dx} = \sqrt{\frac{m\omega}{\hbar}}\, \frac{d}{dy} \qquad \text{— (2)}$$

$$\Rightarrow \frac{d^2}{dx^2} = \left(\frac{m\omega}{\hbar}\right) \frac{d^2}{dy^2} \qquad \text{— (3)}$$

$\Rightarrow$ Equation (1) becomes,

$$\frac{m\omega}{\hbar} \frac{d^2\psi}{dy^2} + \left(\frac{2mE}{\hbar^2} - \frac{m\omega}{\hbar}\, y^2\right)\psi = 0$$

(Multiply by $\frac{\hbar}{m\omega}$)

$$\Rightarrow \boxed{\frac{d^2\psi}{dy^2} + \left(\frac{2E}{\hbar\omega} - y^2\right)\psi = 0} \qquad \text{— (4)}$$

We will solve by iteration, 1st we will try to get an <u>approximate</u> soln. (asymptotic)

y can go upto $\pm\infty$, $\Rightarrow$ when y^2 is large, we can neglect $\left(\frac{2E}{\hbar\omega}\right)$ and <u>approximate it equals 1</u>

Step: 2

$\boxed{0^{th} \text{ iteration}}$

$$\Rightarrow \frac{d^2\psi}{dy^2} = (y^2 - 1)\psi$$

$$\Rightarrow \psi_0(y) = e^{\pm \frac{y^2}{2}}$$

See the logic on P-202

Positive exponent cannot be there

$$\Rightarrow \boxed{\psi_0 = e^{-\frac{y^2}{2}}}$$

0^{th} approximation to solution in order to get form of the solution

Better solution is obtained by variation of parameter,

Let the solution be

$\boxed{1^{st} \text{ iteration}}$

Step III $\psi_1(y) = C\, u(y)\, \psi_0(y)$

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,

$$\frac{d\psi}{dy} = -C y\, e^{-\left(\frac{y^2}{2}\right)} u(y) + C e^{-\frac{y^2}{2}} \left(\frac{du}{dy}\right)$$

$-Cy\, u(y)$

$$\frac{d^2\psi}{dy^2} = -\cancel{C e^{-\frac{y^2}{2}}} + \cancel{C y^2 e^{-\frac{y^2}{2}}}$$

$$+ C e^{-\frac{y^2}{2}} \frac{d^2u}{dy^2} - y\, C \left(\frac{du}{dy}\right) e^{-\frac{y^2}{2}}$$

While deriving write u_y or just u instead of $u(y)$ otherwise confusion can occur !!

$$\frac{d^2\psi}{dy^2} = C e^{-\frac{y^2}{2}} \left[\frac{d^2u}{dy^2} - 2y \frac{du}{dy} + (y^2-1)\, u\right]$$

⊛ Also no need of C while deriving

Hence Putting in ④, we get

$$C e^{-\frac{y^2}{2}} \left[\frac{d^2u}{dy^2} - 2y \frac{du}{dy} + (\cancel{y^2u} - u) + \frac{2E}{\hbar\omega} u - \cancel{y^2 u}\right] = 0$$

$$\Rightarrow C e^{-\frac{y^2}{2}} \left[\frac{d^2u}{dy^2} - 2y\left(\frac{du}{dy}\right) + \left(\frac{2E}{\hbar\omega} - 1\right) u\right] = 0$$

$C \neq 0$, $e^{-\frac{y^2}{2}}$ cannot be 0

$$\Rightarrow \boxed{\frac{d^2u}{dy^2} - 2y\left(\frac{du}{dy}\right) + \underbrace{\left(\frac{2E}{\hbar\omega} - 1\right)} u = 0} \quad — (5)$$

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. $\boxed{\psi_n = (-1)^n e^{y^2} \frac{d^n}{dy^n}\left(e^{-y^2}\right)}$

Step 5

let $\frac{2E_n}{\hbar\omega} - 1 = 2n$

$\frac{2E_n}{\hbar\omega} = (2n+1) \Rightarrow \boxed{E_n = \left(n+\frac{1}{2}\right)\hbar\omega}$

$$\Rightarrow \psi_n(y) = C_n\, U_n(y)\, e^{-\frac{y^2}{2}}$$

Step 4 Power Series Solution of (5) i.e.

$$\frac{d^2u}{dy^2} - 2y\left(\frac{du}{dy}\right) + \left(\frac{2E}{\hbar\omega} - 1\right) u = 0$$

$$U_n(y) = \sum_{0}^{\infty} a_n y^n = a_0 + a_1 y + a_2 y^2 + \ldots\ldots a_n y^n + \ldots\ldots$$

as $n \to \infty$, $a_n \to 0$

i.e. every subsequent coefficient is lesser than previous coefficient. hence $\frac{a_{n+2}}{a_n} \to 0$

$$\frac{du}{dy} = \sum_{n=1}^{\infty} n\, a_n y^{n-1} = \sum_{n=0}^{\infty} n\, a_n y^{n-1}$$ [as @ n=0 term=0

$$\frac{d^2u}{dy^2} = \sum_{n=2}^{\infty} n(n-1)\, a_n y^{n-2} = \sum_{n=0}^{\infty} n(n-1)\, a_n y^{n-2}$$

Substituting in ⑤,

$$\sum_{n=0}^{\infty} n(n-1)\, a_n y^{n-2} - 2y \sum_{n=0}^{\infty} n\, a_n y^{n-1} + \left(\frac{2E}{\hbar\omega} - 1\right) \sum a_n y^n =$$

↑

Put $n' = n-2$

$$\sum_{n'=-2}^{\infty} (n'+2)(n'+1)\, a_{n'+2}\, y^{n'} - \sum 2n\, a_n y^n + \left(\frac{2E}{\hbar\omega} - 1\right) \sum a_n y^n = 0$$

$= n' = 0$ [as $n'+2=0$ @ $n'=-2$; $n'+1=0$ @ $n'=-1$]

$$\sum_{n=0}^{\infty} \left[(n+2)(n+1)\, a_{n+2} + \left(\frac{2E}{\hbar\omega} - 1 - 2n\right) a_n\right] y^n = 0$$

Step 4

NOW if it is true for $\forall n$ $\Rightarrow$ y^n cannot be 0

$$\Rightarrow \frac{a_{n+2}}{a_n} = \frac{\left(2n+1 - \frac{2E_n}{\hbar\omega}\right)}{(n+2)(n+1)}$$

terminate

$$\frac{a_{n+2}}{a_n} = 0$$

Write P_n instead of U_n in final solution

In order that $U_n(y)$ does not diverge, it must be limited till some power of n. $\Rightarrow a_{n+2} = 0$

$\Rightarrow$ n पर condition आ गई !!

$\Rightarrow (2n+1) = \frac{2E}{\hbar\omega}$ $\Rightarrow$ $\boxed{E_n = \left(n + \frac{1}{2}\right)\hbar\omega}$

भले ही n=0,1,2 किसी पर भी valid है !!

$$\boxed{\psi_n(y) = C_n\, u_n(y)\, e^{-\frac{y^2}{2}}}$$

where $U_n(y)$ are hermite's polynomial

$$\boxed{u_n(y) = \frac{(-1)^n}{[redacted]} \, e^{\frac{y^2}{2}} \, \frac{d^n}{dy^n}\left(e^{-y^2}\right)}$$

$u_0(y) = 1$ even

$u_1(y) = 2y$ odd

$u_2(y) = 4y^2 - 2$ even

$u_3(y) = 8y^3 - 12y$ odd

$\vdots$ $\vdots$

Ground state energy

$n = 0$

$$\psi_0(y) = C_0 \, u_0(y) \, e^{-\frac{y^2}{2}}$$

$$\psi_0(y) = C_0 \cdot 1 \cdot e^{-\frac{y^2}{2}} = C_0 e^{-\left(\frac{y^2}{2}\right)}$$

$$\boxed{E_0 = \left(\frac{\hbar\omega}{2}\right)} \quad \boxed{\psi_0(y) = C_0 e^{-\frac{y^2}{2}}} \quad \boxed{= C_0 e^{-\frac{m\omega x^2}{2\hbar}}}$$

1st excited level

$n = 1$

$$u_1(y) = \frac{-1}{[redacted]} \, \cancel{e^{y^2}} \cdot \cancel{e^{-y^2}} \cdot -\cancel{2}y = 2y$$

$$\Rightarrow \boxed{\psi_1(y) = 2C_1 y \, e^{-\left(\frac{y^2}{2}\right)}} \quad \boxed{= 2C_1 \sqrt{\frac{m\omega}{\hbar}} \, x \, e^{-\frac{m\omega x^2}{2\hbar}}}$$

$$\boxed{E_1 = \frac{3}{2}\hbar\omega}$$

Note that C_n's will be calculated using normalization, i.e.

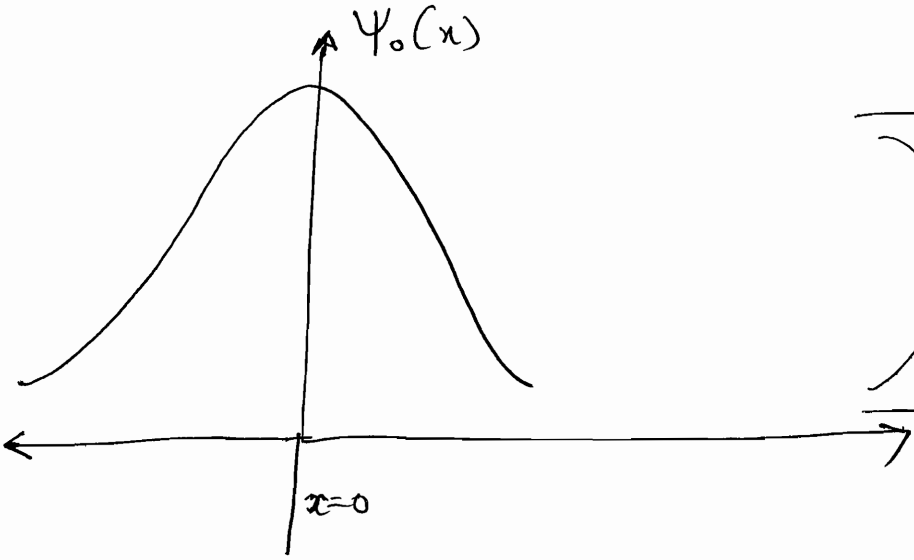
$$|\psi\psi^*| = 1$$

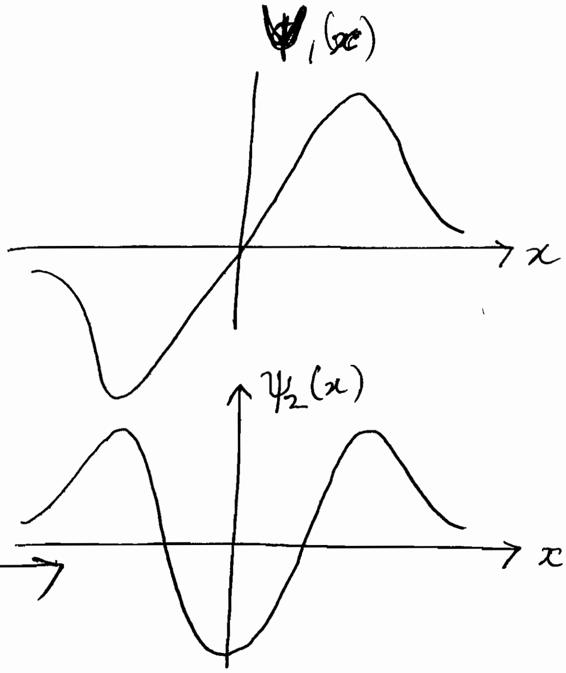
$$C_0^2 \int_{-\infty}^{\infty} e^{-\frac{m\omega x^2}{\hbar}} dx = 1 \qquad \Rightarrow C_0 = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}}$$

$$\Rightarrow C_0^2 \sqrt{\frac{\pi\hbar}{m\omega}} = 1 \checkmark$$

$$\Rightarrow \quad \boxed{\psi_0(x) = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{m\omega}{2\hbar}x^2}}$$

$$\boxed{E_0 = \frac{1}{2}\hbar\omega}$$





$\boxed{\text{Gaussian Wave Function}}$

Probability will also be gaussian !!

Zero Point Energy : $n=0$ $\quad E_0 = \frac{1}{2}\hbar\omega$

Commensurate ~~between~~ with Heisenberg . Uncertainty Principle

Classically, energy can have any values

while

Quantum Oscillator can have ~~any~~ only discrete values of energy $\left(n+\frac{1}{2}\right)\hbar\omega$ $\Rightarrow$ 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 $\left(\frac{\hbar\omega}{2}\right)$ Commensurate with H.U.P..

Classically, Oscillator goes between $\pm a$

a is the turning point where $V = E$

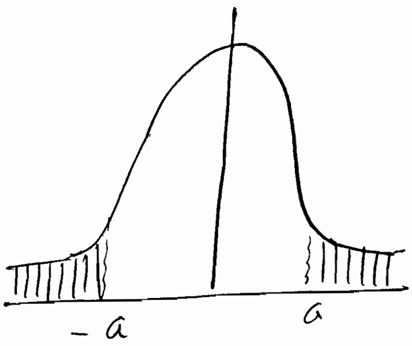
i.e. $\frac{\hbar\omega}{2} = \frac{1}{2} m\omega^2 x^2$

$\Rightarrow a = \pm\sqrt{\frac{\hbar}{m\omega}}$

while

Quantum Mechanically, Oscillator can move from $[-\infty$ to $+\infty]$

eg. 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

$$P_{|x|<a} = \int_{-a}^{a} \psi_0^2(x)\, dx = \sqrt{\frac{m\omega}{\pi\hbar}} \int_{-a}^{a} e^{-\frac{m\omega x^2}{\hbar}}\, dx \quad — (6)$$

$$P_{|x|>a} = 1 - \int_{-a}^{a} \psi_0^2(x)\, dx = 1 - 0.84$$

$$\simeq 16\%$$

To calculate (6)

$$\frac{1}{2} m\omega^2 a^2 = \left(\frac{\hbar\omega}{2}\right)$$

[Classically, Total Energy = Potential Energy]

$$\Rightarrow a = \sqrt{\frac{\hbar}{m\omega}}$$

$$\Rightarrow P_{|x|<a} = \sqrt{\frac{m\omega}{\hbar\pi}} \int_{-\sqrt{\frac{\hbar}{m\omega}}}^{\sqrt{\frac{\hbar}{m\omega}}} e^{-\frac{m\omega}{\hbar}x^2}\, dx$$

Put $\sqrt{\frac{m\omega}{\hbar}}\, x = t \Rightarrow \sqrt{\frac{m\omega}{\hbar}}\, dx = dt$

$$\Rightarrow \boxed{P_{|x|<a} = \frac{1}{\sqrt{\pi}} \int_{-1}^{1} e^{-t^2}\, dt} = \frac{2}{\sqrt{\pi}} \int_0^1 e^{-t^2}\, dt$$

It is an "Error Function".... It cannot be integrated. We can have only approximate values.

$$= \frac{1}{\sqrt{\pi}} \int_{-1}^{1} \left[1 - t^2 + \frac{t^4}{L^2} + \dots\right] dt$$

$$= \frac{1}{\sqrt{\pi}} \left[\left[1 - \frac{t^3}{3} + \frac{t^5}{10}\right]_{-1}^{1} \right]$$

$$\approx \underline{0.84}$$

- 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 $\langle T \rangle = \frac{\langle p_x^2 \rangle}{2m} = \underline{\underline{\left(\frac{\hbar\omega}{4}\right)}}$ ✓

$\langle V \rangle = \frac{1}{2} m\omega^2 \langle x^2 \rangle = \underline{\underline{\frac{1}{4}(\hbar\omega)}}$ ✓

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

$$\left\{ \begin{aligned} \langle x \rangle &= \int \psi^* x \psi \, dx = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{2}} \int_{-\infty}^{\infty} x \, e^{-\frac{m\omega}{\hbar} x^2} dx \\ &= 0 \quad [\text{odd function}] \end{aligned} \right.$$

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

$$\left\{ \langle p_x \rangle = \int_{-\infty}^{\infty} \psi^* \, i\hbar \frac{\partial}{\partial x} \psi \, dx = 0 \quad [\text{odd function}] \right.$$

$\langle x \rangle$: 0 easy
$\langle x^2 \rangle$: ✓ easy
$\langle p_x \rangle$: 0 directly
$\langle p_x^2 \rangle$: use $\langle T \rangle$ easy

$$\langle x^2 \rangle = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{2}} \int_{-\infty}^{\infty} x^2 e^{-\frac{m\omega x^2}{\hbar}} dx$$

$$= \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{2}} 2 \int_{0}^{\infty} x^2 e^{-\left(\frac{m\omega}{\hbar}\right) x^2} dx$$

$$= 2\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{2}} \frac{1}{2\left(\frac{m\omega}{\hbar}\right)^{\frac{3}{2}}} \cdot \Gamma\frac{3}{2}$$

$$= \frac{1}{2}\left(\frac{\hbar}{m\omega}\right)$$

$$\Rightarrow \Delta x \Delta p_x = \sqrt{\frac{\hbar}{2m\omega}} \sqrt{\frac{\hbar m\omega}{2}} = \left(\frac{\hbar}{2}\right)$$

$$\langle p_x^2 \rangle = \frac{\hbar m\omega}{2}$$

$\left[\alpha = \frac{m\omega}{\hbar}\right]$

$$-\hbar^2\left(\frac{\alpha}{\pi}\right)^{\frac{1}{2}} \int_{-\infty}^{\infty} e^{-\frac{\alpha}{2}x^2} \frac{\partial^2}{\partial x^2}\left(e^{-\frac{\alpha x^2}{2}}\right) dx$$

$$= -2\hbar^2\sqrt{\frac{\alpha}{\pi}} \int_0^{\infty} \alpha^2 x^2 e^{-\alpha x^2} - \alpha e^{-\alpha x^2} dx = -2\hbar^2\sqrt{\alpha}\left[\frac{\sqrt{\alpha}}{4} - \frac{\sqrt{\alpha}}{2}\right] = \frac{\hbar^2\alpha}{2} = \left[\frac{\hbar m\omega}{2}\right]$$

(*) Note that for Gaussian Function $\Delta x \Delta p_x$ is minimum i.e. $\left(\frac{\hbar}{2}\right)$

Q 13

Matrix Representation

Refer to lecture 11

$H\psi = E\psi$ [redacted]

$$\Rightarrow H = \left(n + \frac{1}{2}\right)\hbar\omega \, [I]_n$$

$A[I_n][\psi_n] =$ [redacted] $[\psi_n]$

$n \times n$ $\quad n \times 1$ $\quad$ Pure Number $n \times 1$

$$\Rightarrow H = \begin{bmatrix} \frac{1}{2}\hbar\omega & 0 & 0 & 0 & \cdots \\ 0 & \frac{3}{2}\hbar\omega & 0 & 0 & \cdots \\ 0 & 0 & \frac{5}{2}\hbar\omega & 0 & \cdots \\ \cdots & & & & \\ \cdots & & & 0 & \left(n+\frac{1}{2}\right)\hbar\omega \end{bmatrix}$$

$$\psi(x) = \frac{1}{\sqrt{5}}\left\{\psi_0(x) + \sqrt{2}\,\psi_1(x) + \sqrt{2}\,\psi_2(x)\right\}$$

$$\langle\psi|\psi\rangle = 1 = \sum c_i^2$$

$$P_i = |\langle\phi_i|\psi\rangle|^2 = |c_i|^2$$: Probability of state i

$$\langle E \rangle = \langle \psi | H | \psi \rangle$$

$$= \frac{1}{5} \langle \psi_0 | H | \psi_0 \rangle + \frac{2}{5} \langle \psi_1 | H | \psi_1 \rangle + \frac{2}{5} \langle \psi_2 | H | \psi_2 \rangle$$

$$= \frac{1}{5} \times \left(\frac{\hbar\omega}{2}\right) + \frac{2}{5} \times \left(\frac{3\hbar\omega}{2}\right) + \frac{2}{5} \left(\frac{5\hbar\omega}{2}\right)$$

$$= \frac{(1 + 6 + 10)}{10} \hbar\omega = \underline{\underline{\frac{17}{10} \hbar\omega}}$$

Harmonic Oscillator Problem is done !!

(★) do not go into double derivate. 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 $[I_n]$

$[n\times n]$ $[n\times 1]$ $[n\times 1]$

$$\begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix} = a \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix}$$

$$\begin{bmatrix} a & 0 \\ 0 & a \end{bmatrix} \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix} = a \begin{bmatrix} \psi_1 \\ \psi_2 \end{bmatrix}$$

✓ Also, $[A\ B] = AB - BA$

Now, $\underline{\vec{L} = \vec{J} = (\vec{r} \times \vec{p})}$

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

$$= \underline{-i\hbar [\vec{r} \times \vec{\nabla}]} = -i\hbar \begin{bmatrix} i & j & k \\ x & y & z \\ \frac{\partial}{\partial x} & \frac{\partial}{\partial y} & \frac{\partial}{\partial z} \end{bmatrix}$$

$$\Rightarrow J_x = -i\hbar\left[y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right] = YP_z - ZP_y$$

$$J_y = -i\hbar\left[z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right] = ZP_x - XP_z$$

$$J_z = -i\hbar\left[x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right] = XP_y - YP_x$$

Note the cyclic order!!!!

Quantum Mechanics (9)

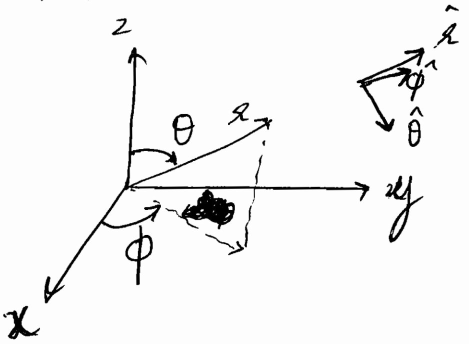
15/02/2012

We have studied $\vec{J} = \vec{r} \times \vec{P} = \vec{r} \times -i\hbar \vec{\nabla}$

$$\Rightarrow \begin{bmatrix} J_x = YP_z - ZP_y \\ J_y = zP_x - xP_z \\ J_z = xP_y - yP_x \end{bmatrix}$$

[redacted]

In (r, θ, ϕ) : spherical coordinates, we have



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

$\rightarrow$ $\hat{r}, \hat{\theta}, \hat{\phi}$ 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 $\hat{\phi}$]

$$= -i\hbar\left[\left[-\frac{1}{\sin\theta}\frac{\partial}{\partial\phi}\right]\hat{\theta} + \left[\frac{\partial}{\partial\theta}\right]\hat{\phi}\right]$$

⊛ $\boxed{\text{Note that no 'r' term in } \vec{L}}$

$\rightarrow$ Note that these are just directions ... operator will operate upon ψ or other function.....

$$\vec{r} = x\hat{i} + y\hat{j} + z\hat{k}$$

$$= r\sin\theta\cos\phi\,\hat{i} + r\sin\theta\sin\phi\,\hat{j} + r\cos\theta\,\hat{k}$$

$$\underline{\hat{r} = \sin\theta\cos\phi\,\hat{i} + \sin\theta\sin\phi\,\hat{j} + \cos\theta\,\hat{k}}$$

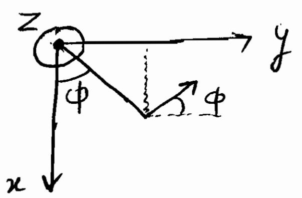
$$\hat{\theta} = \sin(90+\theta)\cos\phi\,\hat{i} + \sin(90+\theta)\sin\phi\,\hat{j} + \cos(90+\theta)\,\hat{k}$$

$$= \underline{\underline{\cos\theta\cos\phi\,\hat{i} + \cos\theta\sin\phi\,\hat{j} - \sin\theta\,\hat{k}}}$$

$$\hat{\phi} = \hat{r}\times\hat{\theta}$$

$$= \underline{\underline{-\sin\phi\,\hat{i} + \cos\phi\,\hat{j}}}$$

[See and write]



Hence, we can write

$$\vec{L} = -i\hbar\left[\frac{\partial}{\partial\theta}\left\{-\sin\phi\,\hat{i} + \cos\phi\,\hat{j}\right\} - \frac{1}{\sin\theta}\frac{\partial}{\partial\phi}\left\{\cos\theta\cos\phi\,\hat{i} + \cos\theta\sin\phi\,\hat{j} - \sin\theta\,\hat{k}\right\}\right]$$

Note that these are not operating on directions

$$= -i\hbar\Big[\left\{-\sin\phi\frac{\partial}{\partial\theta} - \frac{1}{\sin\theta}\cos\theta\cos\phi\frac{\partial}{\partial\phi}\right\}\hat{i}$$

$$+ \left\{\cos\phi\frac{\partial}{\partial\theta} - \frac{\cos\theta\sin\phi}{\sin\theta}\frac{\partial}{\partial\phi}\right\}\hat{j}$$

$$+ \left\{\frac{\partial}{\partial\phi}\right\}\hat{k}\Big]$$

$$L_x = -i\hbar \left[-\sin\phi \frac{\partial}{\partial\theta} - \cot\theta \cos\phi \frac{\partial}{\partial\phi} \right]$$

$$L_y = -i\hbar \left[\cos\phi \frac{\partial}{\partial\theta} - \cot\theta \sin\phi \frac{\partial}{\partial\phi} \right]$$

$$L_z = -i\hbar \left[\frac{\partial}{\partial\phi} \right]$$

★ L Operator in spherical Coordinates

$$\vec{L}\cdot\vec{L} = L_x^2 + L_y^2 + L_z^2$$

$$\Rightarrow L^2 = -\hbar^2 \left[\left(\frac{1}{\sin\theta}\right) \frac{\partial}{\partial\theta}\left(\sin\theta \frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} \right]$$

⊙ Note that they are operators and not numbers
$L_x^2 = L_x(L_x)$

We know

$$\nabla^2 = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right) + \frac{1}{r^2 \sin^2\theta}\frac{\partial^2}{\partial\phi^2} + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta \frac{\partial}{\partial\theta}\right)$$

laplacian

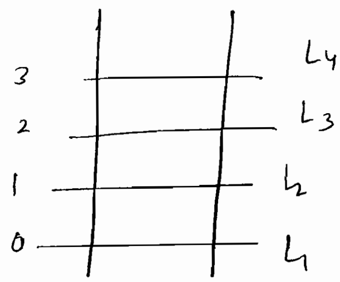
$$= \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{1}{r^2}\frac{L^2}{\hbar^2}$$

$$\boxed{L^2 = -\hbar^2 r^2 \left[\nabla^2 - \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial}{\partial r}\right) \right]}$$

$$\boxed{L_x \pm i L_y = L_\pm}$$

L_+ Operator takes the angular momentum to next quantized level.

L_- Operator takes it 1 level below.



→ Quantum Mechanical values of L ⇒ Quantized steps
i.e. Particle in particular states

$$\left\{ L_{\pm} = \pm \hbar e^{\pm i\phi} \left[\frac{\partial}{\partial\theta} \pm i\cot\theta \frac{\partial}{\partial\phi} \right] \right\}$$

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,

$$\boxed{L^2 Y(\theta,\phi) = \lambda\hbar^2 Y(\theta,\phi)}$$

Angular Momentum Problem

- Note that in order to determine L, we can determine L^2 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) $L^2 \; Y(\theta,\phi) = \lambda \hbar^2 \; Y(\theta,\phi)$

eigenvalue $\boxed{L^2 = \lambda \hbar^2}$

Angular Momentum Magnitude Quantization

$\Rightarrow |\vec{L}| = \sqrt{\lambda}\,\hbar$

(ii) $\boxed{L_z Y(\theta,\phi) = \lambda' \hbar \; Y(\theta,\phi)}$ Space Quantization of Angular Momentum

⊙ So our aim is to find λ, λ' and $Y(\theta,\phi)$

We can combine the 2 as,

$$[L^2, L_z] \; |Y(\theta,\phi)\rangle = 0$$

✓ same eigenfunction for both

$\Rightarrow$ commuting operators

$\Rightarrow$ Commutator $= 0$

$$[L^2, L_z] = 0$$

Simultaneous measurement is possible i.e. same ψ.

$$\left.\begin{aligned} [L^2 \; L_x] &= 0 \\ [L^2 \; L_y] &= 0 \\ [L^2 \; L_z] &= 0 \end{aligned}\right\}$$

any 1 of the 3

$\rightarrow$ 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.

$$L_z Y(\theta,\phi) = \lambda' \hbar \, Y(\theta,\phi)$$

$$\boxed{-i\hbar \frac{\partial}{\partial \phi} Y = \lambda' \hbar Y}$$

Put $\Theta(\theta)\,\Phi(\phi) = Y(\theta,\phi)$

Solving it w/o separating the variables is WRONG !!

$$\Rightarrow \frac{\partial}{\partial\phi} Y = i\lambda' Y$$

$$\Rightarrow \cancel{\Theta(\theta)} \cdot \frac{\partial \Phi}{\partial \phi} = i\lambda' \cancel{\Theta(\theta)}\, \Phi(\phi)$$

$$\frac{d\Phi}{d\phi} = i\lambda'\Phi$$

$$\Rightarrow \ln\Phi = i\lambda'\phi + A'$$

$$\Rightarrow \Phi = A e^{i\lambda'\phi}$$

$$\Rightarrow \boxed{\Phi = A e^{i\lambda'\phi}} \quad \text{--- (1)}$$

$$\langle \Phi | \Phi \rangle = 1$$

$$\Rightarrow \int_0^{2\pi} |A|^2 e^{-i\lambda'\phi} e^{i\lambda'\phi} \, d\phi = 1$$

$$\Rightarrow |A|^2 \cdot 2\pi = 1$$

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

Now we know $\Phi(\phi + 2\pi) = \Phi(\phi)$

[Wave function must be single valued]

$$\Rightarrow \frac{1}{\sqrt{2\pi}} e^{i\lambda'(\phi+2\pi)} = \frac{1}{\sqrt{2\pi}} e^{i\lambda'\phi}$$

$\Rightarrow \quad e^{i(2\pi\lambda')} = 1$

$\Rightarrow \quad \cos(2\pi\lambda') = 1$

$\Rightarrow \quad 2\pi\lambda' = 2n\pi$

$\Rightarrow \quad \boxed{\lambda' = n} \qquad n = 0, \pm 1, \pm 2, \pm 3 \ldots\ldots$

Hence λ' is an integer

$= m_\ell$: Angular Momentum Quantum Number.

★ From this part we got to know, that λ_z is the coefficient m_ℓ of $(i\phi)$ in exponent of $\Phi(\phi)$. We should have done this part after calculating $\Phi(\phi)$ done in part II .....

$\Rightarrow \quad \boxed{L_z = m_\ell \hbar}$ Eigen Values of L_z

Now solving 1^{st} part of Angular Momentum Problem,

$$L^2 Y(\theta, \phi) = \lambda \hbar^2 Y(\theta, \phi)$$

$$\left[\frac{1}{\sin\theta} \frac{\partial}{\partial\theta}\left(\sin\theta \frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2}\right] Y = -\lambda Y$$

Put $\quad Y(\theta, \phi) = \Theta(\theta) \, \Phi(\phi)$

$$\Rightarrow \quad \frac{\Phi}{\sin\theta} \frac{\partial}{\partial\theta}\left[\sin\Theta \frac{\partial \Theta}{\partial\theta}\right] + \frac{\Theta}{\sin^2\theta} \frac{d^2\Phi}{d\phi^2} = -\lambda \Theta \Phi$$

divide by $\Theta\Phi$

$$\Rightarrow \quad \frac{1}{\Theta \sin\theta} \frac{d}{d\theta}\left[\sin\theta \frac{d\Theta}{d\theta}\right] + \frac{1}{\sin^2\theta \, \Phi} \frac{d^2\Phi}{d\phi^2} = -\lambda$$

Multiply by $\sin^2\theta$

$$\Rightarrow \quad \frac{\sin\theta}{\Theta} \frac{d}{d\theta}\left[\sin\theta \frac{d\Theta}{d\theta}\right] + \lambda \sin^2\theta = -\frac{1}{\Phi} \frac{d^2\Phi}{d\phi^2} = m_\ell^2$$

(From eqn (1) on last page)

LHS : $f(\theta)$

RHS : $f(\phi)$

Hence both are const.

$\Rightarrow$ let them be m_ℓ^2

→ 2nd easier way is to 1st find eigenvalues & eigenfunctions of L_z and then use them in L^2 as $[L^2, L_z] = 0$ $\Rightarrow$ they will have a complete set of common eigenfunctions.

$$-\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2} = m_\ell^2$$

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

$$\boxed{\frac{\sin\theta}{\Theta}\frac{d}{d\theta}\left(\sin\theta \frac{d\Theta}{d\theta}\right) + \left(\lambda \sin^2\theta - m_\ell^2\right) = 0}$$

~~Legendre Differential Equation~~

let $\boxed{\cos\theta = x}$

$\Rightarrow$ $-\sin\theta \, d\theta = dx$

$$\frac{d}{d\theta} = \frac{d}{dx}\cdot\frac{dx}{d\theta} = -\sin\theta \frac{d}{dx}$$

First substitute and then do the derivative!! so that you do not have to derive for $\left(\frac{d^2}{d\theta^2}\right)$

$$-\frac{\sin^2\theta}{\Theta}\frac{d}{dx}\left(-\sin^2\theta \frac{d\Theta}{dx}\right) + \left(\lambda \sin^2\theta - m_\ell^2\right) = 0$$

$$\Rightarrow (1-x^2)\frac{d}{dx}\left((1-x^2)\frac{d\Theta}{dx}\right) + \left[\lambda(1-x^2) - m_\ell^2\right]\Theta = 0$$

$$\Rightarrow (1-x^2)\frac{d}{dx}\left((1-x^2)\frac{d\Theta}{dx}\right) + \left(\lambda(1-x^2) - m_\ell^2\right)\Theta = 0$$

differentiating & dividing by $(1-x^2)$ (not necessary if not multiplied by $\sin^2\theta$, if doing in above manner)

$$\boxed{(1-x^2)\frac{d^2\Theta}{dx^2} - 2x\frac{d\Theta}{dx} + \left[\lambda - \frac{m_\ell^2}{(1-x^2)}\right]\Theta = 0}$$

It is Associated Legendre's Differential Equation

This is worked out by Power Series Method.

$\Theta(x)$ = Solutions are Associated legendre's polynomials.

$$\Theta(x) = B \; P_\ell^{m_\ell}(x)$$

If $m_\ell = 0$ $\Rightarrow$ Legendre's Differential Equation

$$(1-x^2)\frac{d^2\Theta}{dx^2} - 2x\frac{d\Theta}{dx} + \lambda\Theta = 0$$

[Θ तो आ गया ... λ निकालने के लिए Power Series method]

Solution by Power Series Method

Let $\Theta(x) = \sum_{\ell=0}^{\infty} a_\ell x^\ell = a_0 + a_1 x + a_2 x^2 + \ldots$

Note that $a_\ell \to 0$ as $x \to \infty$

$$\frac{d\Theta}{dx} = a_1 + 2a_2 x + \ldots = \sum_{\ell=1}^{\infty} a_\ell \, \ell \, x^{\ell-1}$$

$$\frac{d^2\Theta}{dx^2} = 2a_2 + 3.2\,a_3 x + \ldots = \sum_{\ell=2}^{\infty} a_\ell \, \ell(\ell-1) \, x^{\ell-2}$$

$$\Rightarrow \sum (1-x^2)\, a_\ell \, \ell(\ell-1)\, x^{\ell-2} - \sum 2x\, \ell\, a_\ell\, x^{\ell-1} + \lambda \sum a_\ell x^\ell = 0$$

[do not touch the coefficient a_ℓ while differentiating]

$$\Rightarrow \sum l(l-1)\, a_l\, x^{l-2} - \sum a_l\, l(l-1)\, x^l$$

$$- \sum 2 l a_l\, x^l + \sum \lambda\, a_l\, x^l = 0$$

Put $l' = l+2$

$$\Rightarrow \sum (l'+2)(l'+1)\, a_{l'+2}\, x^l \quad : \quad 1^{st} \text{ term}$$

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 diverse. $\therefore$ must truncate ~~after~~ after some value, say l

$$\frac{a_{l+2}}{a_l} \quad 0$$

$$\Rightarrow l(l+1) - \lambda = 0$$

$$\Rightarrow \boxed{\lambda = l(l+1)}$$

$$\& \ \Theta(x) = \Theta^l(x) = \frac{1}{2^l\, \underline{|l}} \frac{d^l}{dx^l} (x^2-1)^l = P_l(x)$$

$$\Theta^0(x) = 1$$
$$\Theta^1(x) = x$$
$$\Theta^2(x) = \frac{(3x^2 - 1)}{2}$$

} Legendre's Polynomials.

But this was calculated for $m_l = 0$ → Legendre's Polynomial $P_l(x)$ are polynomials of degree 'l'.

But in general m_l may not be 0

In such a case,

$$\lambda = l(l+1)$$

and $\quad |m| \leq l$

Associated Legendre's Polynomials are m^{th} derivatives of Legendre's Polynomial

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

$\Rightarrow$ if $|m| > l$ solution $= 0$

Now,

$$\Theta(x) = \underbrace{B \, P_l^{m_l}(x)}_{\text{Associated Legendre's Polynomials}} \qquad \Rightarrow \boxed{|m| \leq l}$$

Associated Legendre's Polynomial

$$= B \left[\frac{d^{|m|}}{dx^{|m|}} P_l(x) \right] (1 - x^2)^{\frac{|m|}{2}}$$

Legendre's Polynomial

← I am not interested in precise value. I just want to know that there are $|m|$ derivatives.

Hence,

$$L^2 Y(\theta, \phi) = l(l+1) \hbar^2 \, Y(\theta, \phi) \quad ; \quad l = 0, 1, 2, \dots$$

$\Rightarrow$ Eigen Values $\quad L^2 = l(l+1)\hbar^2$

$$\Rightarrow L = 0, \sqrt{2}\hbar, \sqrt{6}\hbar, \sqrt{12}\hbar$$

Eigen Function $\quad Y(\theta, \phi) = B \, P_l^m(\cos\theta) \, e^{im_l\phi}$

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

$P_l^m(x) = P_l^m(\cos\theta)$ as $x = \cos\theta$

Writing the solutions for 1st 3 states :

~~s state~~

$l = 0 \qquad m_l = 0$

$L^2 = 0 \qquad L_z = 0$ } no significance

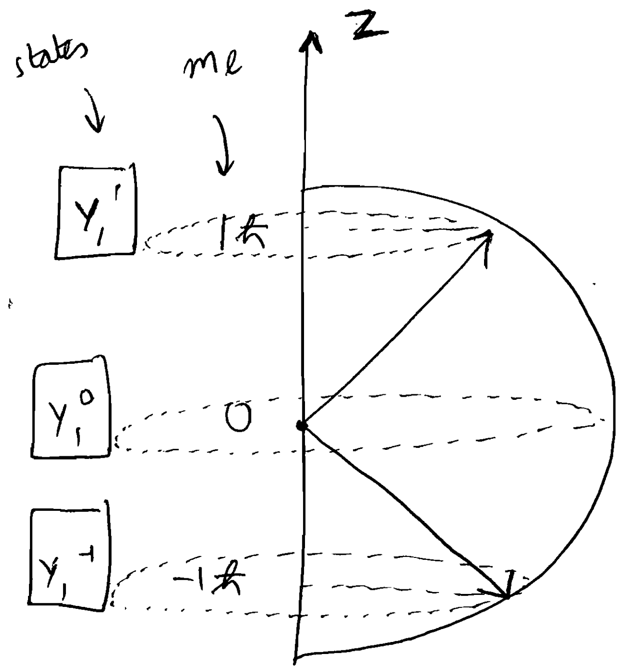
~~p th state~~

$l = 1 \qquad L = \sqrt{2}\,\hbar$

$m_l = 0, 1, -1$: 3 possible states p_x, p_y, p_z

$L_z = 1\hbar, -1\hbar, 0$

Space Quantization of Angular Momentum



$L = l = \sqrt{2}\,\hbar$ (say)

also called p th substate

Hence Angular Momentum Vector can take only discrete orientation

$$Y(\theta,\phi) = P_l^{m_l}\cos\theta \; e^{im_l\phi}$$

$$P_l^{m_l}\cos\theta = \frac{d^{|m|}}{dx^{|m|}}(x^2-1) = \begin{cases}(x^2-1), & m=0\\ (2x), & m=\pm 1\end{cases}$$

$$Y_1^0 = \cos\theta\, e^{i(0)} = \cos\theta$$

$$Y_1^1 = \cos\theta\, e^{i\phi}$$

$$Y_1^{-1} = \cos\theta\, e^{-i\phi}$$

(d state)

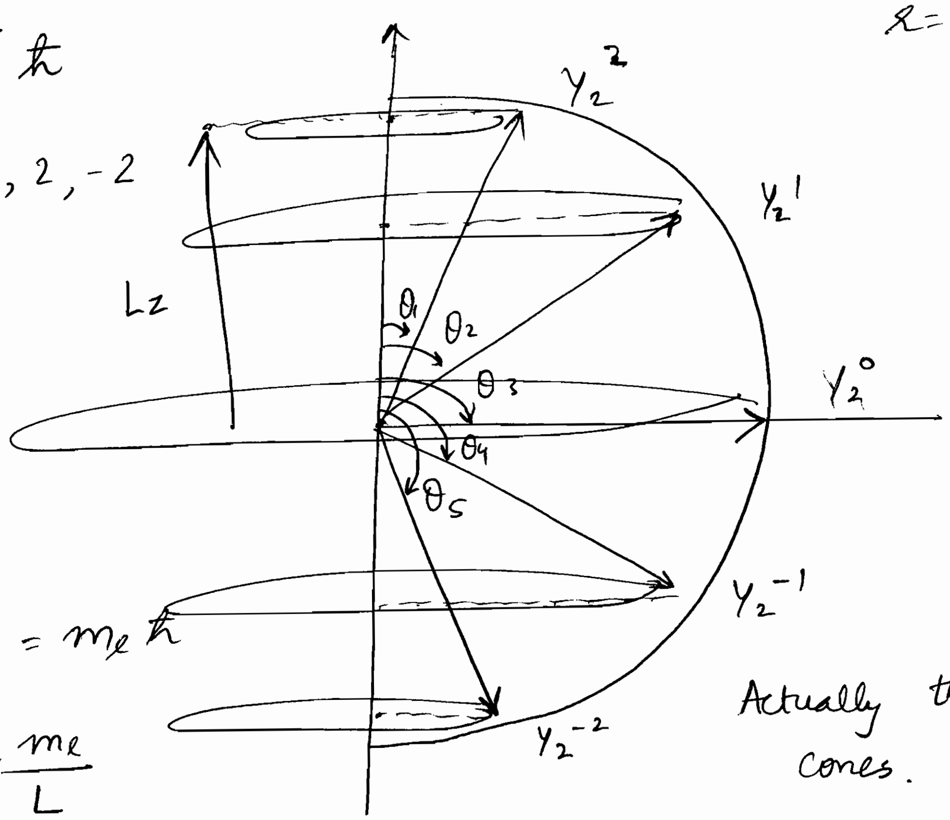
$l = 2$ $\quad d_{xy}, d_{yz}, d_{xz}, d_{x^2-y^2}, d_{z^2}$.

$L^2 = 6\hbar^2$

$L = \sqrt{6}\hbar$

$r = L = \sqrt{6}\hbar$

$m_l = 0, 1, -1, 2, -2$



$L_z = L\cos\theta = m_l\hbar$

$\cos\theta = \dfrac{\hbar m_l}{L}$

Actually they are cones.

$\theta_1 = \cos^{-1}\left(\dfrac{2}{\sqrt{6}}\right)$

$\theta_2 = \cos^{-1}\left(\dfrac{1}{\sqrt{6}}\right)$

$\theta_3 = \cos^{-1} 0 = \dfrac{\pi}{2}$

$\theta_4 = \cos^{-1}\left(\dfrac{-1}{\sqrt{6}}\right)$

$\theta_5 = \cos^{-1}\left(\dfrac{2}{\sqrt{6}}\right)$

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)

16/02/2

In the last class, we have done Angular Momentum Problem

$$\boxed{L^2 Y(\theta,\phi) = l(l+1)\hbar^2\, Y(\theta,\phi) \qquad l = 0, 1, 2, \ldots}$$

$$\boxed{L_z Y(\theta,\phi) = m_l \hbar\, Y(\theta,\phi) \qquad m_l = 0, \pm 1, \pm 2, \ldots \pm l}$$

For a particular l, we will have $(2l+1)$ values of m_l, hence $(2l+1)$ states for given l.

Magnitude Quantization $\Rightarrow$ $L^2 = l(l+1)\hbar^2$

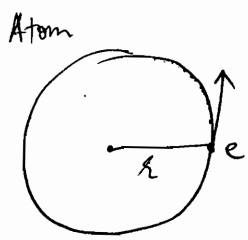
Space Quantization $\Rightarrow$ $L_z = m_l\hbar$

$\Rightarrow$ along a particular direction, L can take only specific values.

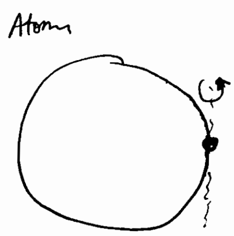
(*) ∞-fold degeneracy as I can associate $f(r)$ (any) to $\psi(r,\theta,\phi)$ as $\psi = f(r)\, Y_l^m(\theta,\phi)$ ....

$$\boxed{Y_l^{m_l}(\theta,\phi) = B\, P_l^{m_l}(\cos\theta)\, e^{i m_l \phi}}$$

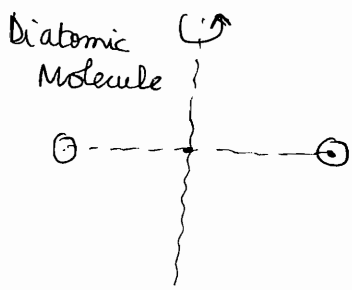
(*) Angular Momentum is not only quantized in magnitude but also quantized in space !!



L due to orbital motion

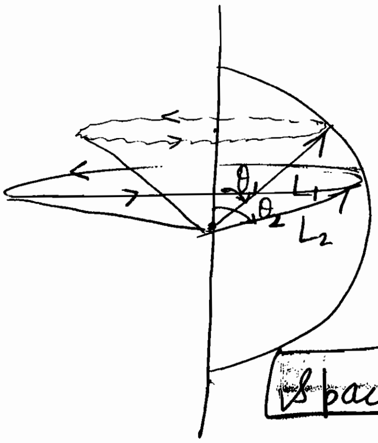


L due to spin motion



⊙ Angular Momentum is also quantized in Nucleus.

Precession : Rotation of Angular Momentum



Note that it is example of Precession.

Space Quantization of Angular Momentum

Orbital	s	p	d	f	g
l	0	1	2	3	4
L^2	0	$2\hbar^2$	$6\hbar^2$	$12\hbar^2$	$20\hbar^2$

in 'd' orbital

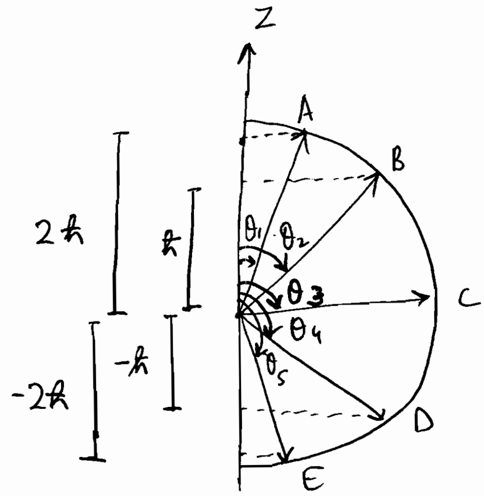
$l = 2$

$L^2 = 6\hbar^2 \Rightarrow L = \sqrt{6}\hbar$

No. of orientations $= (2l+1) = 5$ $\quad d_{xy} \quad d_{xy} \quad d_{xz} \quad d_{x^2-y^2} \quad d_{z^2}$

$= m_l \hbar$

$= 0, \pm 1\hbar, \pm 2\hbar$



A : $L_z = 2\hbar = L\cos\theta_1 \Rightarrow \theta_1 = \cos^{-1}\left(\frac{2}{\sqrt{6}}\right)$

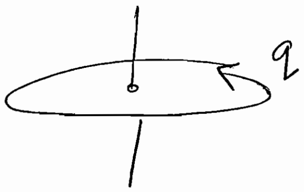
B : $L_z = \hbar = L\cos\theta_2 \Rightarrow \theta_2 = \cos^{-1}\left(\frac{1}{\sqrt{6}}\right)$

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.



$$\boxed{I = \left(\frac{q}{\tau}\right) = q\nu = \frac{q\omega}{2\pi}}$$

- Electron, Proton, Neutron are $\frac{1}{2}$ spin particles.

Every current carrying loop is equivalent to a magnetic dipole.

$$B = \frac{\mu_0 I}{2r} \; ; \quad \boxed{\vec{\mu} = I\vec{A}} \quad = \frac{q\omega}{2\pi}\pi r^2$$

↑ dipole moment

$$= \left(\frac{q\omega r^2}{2}\right)$$

$$= \frac{mq\omega r^2}{2m}$$

$$= \boxed{\left(\frac{q}{2m}\right)\vec{L}}$$

✓ If ⊕vely charged particle, μ and L are in same direction.

✓ If ⊖vely charged particle, μ and L are opposite.

✓ If a charge particle has angular momentum ⇒ it has a dipole moment.

Now every atom has rotating charged particles, ⇒ it has intrinsic magnetic field.

$$\tau = \vec{\mu} \times \vec{B}$$

- Hence this is the reason of observed rotation of $\vec{L}$!!

Torque tries to rotate $\vec{\mu}$ in direction of field.

⇒ Torque will rotate $\vec{L}$; hence precession of Angular Momentum

$$\vec{\tau} = \vec{\mu} \times \vec{B}$$

$$\frac{dL}{dt} = \frac{q\vec{L}}{2m} \times \vec{B}$$: 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 $L=0$

eg. $_{26}$Iron : $\boxed{1s^2\, 2s^2\, 2p^6\, 3s^2\, 3p^6\, 3d^6\, 4s^2}$

For them $$\boxed{\frac{\text{Spin Magnetic Moment}}{\text{Spin Angular Momentum}} = \left(\frac{q}{m}\right)}$$ ✓

Hence, classically we were not able to explain gyromagnetic ratio. We need quantum mechanical concept of spin to explain this.

Spin Angular Momentum

$$\boxed{S^2 = s(s+1)\,\hbar^2}$$

$S_z = m_s \hbar$

$m_s : \; -s$ to $+s$

$= \left(\frac{-1}{2}, \frac{1}{2}\right)$ for electron

Why spin to be introduced?

1) To explain Gyromagnetic ratio of Ferromagnetic materials $(l=0)$

$= \left|\frac{\mu}{s}\right| = \left(\frac{e}{m}\right)$

→ These are called 'Pre Spin' Riddles

2) Fine structure of spectral lines

3) Zeeman Effect

4) Stern - Gerlach Experiment [This experiment fixes $s = \left(\frac{1}{2}\right)$ for electron]

5) Also apart from $0, 2\hbar^2, 6\hbar^2, 12\hbar^2 \ldots\ldots$, we have also observed values of angular momentum like

$\frac{3}{4}\hbar^2$, $\frac{15}{4}\hbar^2 \ldots\ldots$

$\left(s = \frac{1}{2}\right)$ $\quad \left(s = \frac{3}{2}\right)$

Hence spin required to explain this.

⊙ Since 's' values are quantized, it is not a simple classical motion but rather a quantum mechanical concept.

Gaud Smidt and Uhlenbeck proposed in 1925 the idea of spin for particles.
[15p के Postcard पे अमर हो गए]

Properties of Angular Momentum

(1)
$$\vec{L} \times \vec{L} = i\hbar \vec{L}$$
$$\vec{S} \times \vec{S} = i\hbar \vec{S}$$
$$\vec{J} \times \vec{J} = i\hbar \vec{J}$$
$$\vec{I} \times \vec{I} = i\hbar \vec{I}$$

⊛ 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:

$$\boxed{\begin{aligned} [L_x, L_y] &= i\hbar L_z \\ [L_y\ L_z] &= i\hbar L_x \\ [L_z\ L_x] &= i\hbar L_y \end{aligned}}$$

Note that the 3 are cyclic results

Commutation Result satisfied by Angular Momentum Operators.

Cross Product expansion में 2nd row variable is multiplied to 3rd row variable and never vice versa.

$$\begin{vmatrix} i & j & k \\ a_1 & a_2 & a_3 \\ b_1 & b_2 & b_3 \end{vmatrix} = \begin{aligned} & i(a_2b_3 - a_3b_2) \\ & + j(a_3b_1 - a_1b_3) \\ & + k(a_1b_2 - a_2b_1) \end{aligned}$$

$$\begin{vmatrix} \hat{i} & \hat{j} & \hat{k} \\ L_x & L_y & L_z \\ L_x & L_y & L_z \end{vmatrix} \Rightarrow \hat{i}\,[L_y L_z - L_z L_y] + \hat{j}\,[L_z L_x - L_x L_z] + \hat{k}\,[L_x L_y - L_y L_x]$$

$$= i\hbar\,[L_x\,\hat{i} + L_y\,\hat{j} + L_z\,\hat{k}]$$

NOTED FOR 1st TIME IN LIFE .... 2nd TERM OF CROSS PRODUCT IS NOT NEGATIVE OR OPPOSITE .... ITS SIMPLY THE NEXT TWO ROWS 3rd and 1st are PLACED OPPOSITE

NOTE THAT CYCLIC ORDER IS FOLLOWED

$$\Rightarrow \quad L_y L_z - L_z L_y = i\hbar L_x$$

$$L_z L_x - L_x L_z = i\hbar L_y$$

$$L_x L_y - L_y L_x = i\hbar L_z$$

✓ 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 $[L_x \; L_y] = i\hbar L_z$

✓ No need to open into derivatives just use $[AB, C]$ and $[A, BC]$ Properties repeatedly along with $[x \; P_x] = i\hbar$

$$\text{L.H.S.} = L_x L_y - L_y L_x$$

$$L_x L_y = -\hbar^2\left[y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right]\left[z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right]$$

$$L_y L_x = -\hbar^2\left[\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)\right]$$

$$L_x L_y = -\hbar^2\left(y\frac{\partial}{\partial z}\left(z\frac{\partial}{\partial x}\right) - y\frac{\partial}{\partial z}\left(x\frac{\partial}{\partial z}\right) - z\frac{\partial}{\partial y}\left(z\frac{\partial}{\partial x}\right) + z\frac{\partial}{\partial y}\left(x\frac{\partial}{\partial z}\right.\right.$$

$$= -\hbar^2\left[y\frac{\partial}{\partial x} + \cancel{yz\frac{\partial^2}{\partial z\,\partial x}} - \cancel{xy\frac{\partial^2}{\partial z^2}} - \cancel{z^2\frac{\partial^2}{\partial x\,\partial y}} + \cancel{xz\frac{\partial^2}{\partial y\,\partial z}}\right]$$

$$L_y L_x = -\hbar^2\left[z\frac{\partial}{\partial x}\left(y\frac{\partial}{\partial z}\right) - z\frac{\partial}{\partial x}\left(z\frac{\partial}{\partial y}\right) - x\frac{\partial}{\partial z}\left(y\frac{\partial}{\partial z}\right) + \frac{x\partial}{\partial z}\left(\frac{z\partial}{\partial y}\right)\right]$$

$$= -\hbar^2\left[\cancel{zy\frac{\partial^2}{\partial x \partial z}} - \cancel{z^2\frac{\partial^2}{\partial x \partial y}} - \cancel{xy\frac{\partial^2}{\partial z^2}} + x\frac{\partial}{\partial y} + \cancel{xz\frac{\partial^2}{\partial z \partial y}}\right]$$

Substracting,

$$[L_x \; L_y] = -\hbar^2\left[y\frac{\partial}{\partial x} - x\frac{\partial}{\partial y}\right]$$

$$= \frac{\cancel{+}\hbar^2(-L_z)}{\cancel{-}i\hbar}$$

$$= i\hbar L_z$$

$$= \text{R.H.S}$$

Hence, Proved.

Similar relation: $[S_x \; S_y] = i\hbar S_z$

In Matrix $[A\;B, C] = A[B, C] + [A, C]B$

(2) $[L^2 \quad L_x] = 0$

$[L^2 \quad L_y] = 0$

$[L^2 \quad L_z] = 0$

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 $|\vec{L}|$ with same accuracy.
Error will be there in other 2 components.

Physical interpretatio

$$A^2A = AA^2 = A^3 \quad \text{(in matrix)}$$

$$[L^2, L_z] = 0 \quad \text{(To prove)}$$

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....

$$= L_x[L_x \; L_z] + [L_x \; L_z]L_x + L_y[L_y, L_z] + [L_y \; L_z]L_y$$

$$= \cancel{L_x(-i\hbar L_y)} + \cancel{-i\hbar L_y L_x} + \cancel{L_y\, i\hbar L_x} + \cancel{i\hbar L_x L_y}$$

$$= 0$$

$$= \text{R.H.S.}$$

We can write:

$$\boxed{[L^2, L_z]\underbrace{|l,m\rangle}_{\psi(l,m)} = 0}$$

$\psi(l,m)$: state representation of Angular Momentum

$[X, P_x] |\psi\rangle$

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

$= -ix\hbar\cancel{\left(\frac{\partial \psi}{\partial x}\right)} + i\hbar\psi + i\hbar x\cancel{\left(\frac{\partial \psi}{\partial x}\right)}$

$= i\hbar|\psi\rangle$

$\Rightarrow \boxed{[x \quad P_x] |\psi\rangle = i\hbar|\psi\rangle}$

Hence, it means x, P_x cannot be simultaneously measured with similar level of accuracy.

$[X^2, P_x] |\psi\rangle = 2i\hbar X |\psi\rangle$

$\boxed{[X^n, P_x] |\psi\rangle = n i\hbar X^{n-1} |\psi\rangle}$ ✓ Perfect 1 line proof

Similarly

$\boxed{[X, P_x{}^m] |\psi\rangle = m i\hbar P_x{}^{m-1}}$ ✓ Perfect Proof by induction

$[L_x, x]\psi = ? = \text{say, } \lambda\psi$

$L_x x\psi - x L_x\psi$

$= -i\hbar\left[\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)(x\psi)\right] + x i\hbar\left[y\frac{\partial}{\partial z}\psi - z\frac{\partial \psi}{\partial y}\right]$

$= \underline{0}$

$$\boxed{[L_x , x] = 0} \quad \leftarrow \text{can be measured simultaneously}$$

$$[L_x , y] \neq 0 \quad \leftarrow \text{cannot be measured simultaneously}$$

$$\boxed{[L_x , y] = i\hbar z}$$

★ 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 commutating eigenfunctions for a n-level degeneracy.

Quantum Physics (11) 17/02/12

Ladder Operations

$L_+ = L_x + iL_y$

$L_- = L_x - iL_y$

⊛ $L_{(+)}$ and $L_{(-)}$ are not hermitian operators but adjoints of each other
ie. $\langle L_{(+)}\psi_1 | \psi_2\rangle = \langle \psi_1 | L_{(-)}\psi_2\rangle$
& $\langle L_{(-)}\psi_1 | \psi_2\rangle = \langle \psi_1 | L_{(+)}\psi_2\rangle$

$$\boxed{[L^2, L_+] = 0 = [L^2, L_-]} \quad \text{— (1)}$$

used to show l same

$$\boxed{L_\pm : \text{Ladder Operators}}$$

3 Properties of adjoints
① $(A^{ad})^{ad} = A$
② $(AB)^{ad} = B^{ad}A^{ad}$
③ $(A+B)^{ad} = A^{ad} + B^{ad}$

$[L^2, L_+] = [L^2\ L_x] + i[L^2\ L_y] = 0 + 0 = 0$

$[L^2, L_{(-)}] = [L^2\ L_x] - i[L^2\ L_y] = 0 - 0 = 0$

○ Bra $\langle\psi_1|$:- Symbol to indicate the 1st function in a scalar product of state $|\psi_1\rangle$ with $|\psi_2\rangle$.

$$\langle\psi_1|\psi_2\rangle = \int_{space} \psi_1^* \psi_2 \, dx$$

The scalar product is NON COMMUTATIVE.

Now,

$[L_+, L_z]$

$= [L_x + iL_y, L_z]$

$= [L_x\ L_z] + i[L_y\ L_z]$

$= -i\hbar L_y + i\, i\hbar L_x$

$= -\hbar L_+$

i.e.

$$\boxed{[L_z, L_+] = \hbar L_+}$$

used to m+1 or m-1

Similarly,

$$\boxed{[L_z, L_-] = -\hbar L_-}$$

⊙ If $|\psi\rangle = c_1[i|\alpha\rangle + 2|\beta\rangle]$
where $|\alpha\rangle$ and $|\beta\rangle$ are orthonormal wave functions

$\Rightarrow \langle\psi| = c_1[-i\langle\alpha| + 2\langle\beta|] = (|\psi\rangle)^*$

and

$|\phi\rangle = c_2[|\alpha\rangle - i|\beta\rangle]$

$\Rightarrow \langle\psi|\phi\rangle$

$= \langle\psi| * |\phi\rangle$

$= c_1[-i\langle\alpha| + 2\langle\beta|] * [c_2(|\alpha\rangle - i|\beta\rangle)]$

$= c_1c_2[-i\langle\alpha|\alpha\rangle - 2i\langle\beta|\beta\rangle]$

$= \underline{-3i\, c_1 c_2}$

Also, since $L_+ = L_x + iL_y$

and $L_- = L_x - iL_y$

$$\begin{cases} \langle L_{(+)}\psi_1|\psi_2\rangle = \langle \psi_1| L_{(-)}\psi_2\rangle \\ \langle L_{(-)}\psi_1|\psi_2\rangle = \langle \psi_1| L_{(+)}\psi_2\rangle \end{cases}$$

★ $\langle \psi_1|A|\psi_2\rangle$ normally means

$\langle \psi_1|(A\psi_2)\rangle = \int_{space} \psi_1^* (A\psi_2)\, dx$

For Hermitian operators only,

$\langle \psi_1 | A\psi_2\rangle = \langle A\psi_1 | \psi_2\rangle$

$= \int_{space} (A\psi_1)^* \psi_2 \, dx$

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 $|l, m\rangle$

$$\Rightarrow [L_z \;\; L_+]|l,m\rangle = \hbar L_+ |l,m\rangle$$

$$\Rightarrow L_z L_{(+)} |l,m\rangle - L_{(+)} \underbrace{L_z |l,m\rangle} = \hbar L_{(+)} |l,m\rangle$$

$$\Rightarrow L_z \;\; L_+|l,m\rangle - L_{(+)} m_l \hbar \;|l,m\rangle = \hbar L_{(+)} |l,m\rangle$$

$$\Rightarrow \boxed{L_z\left[\underbrace{L_{(+)}|l,m\rangle}\right] = \hbar(m_l+1)\left[\underbrace{L_+|l,m\rangle}\right]}$$

Also from ①

$L^2 [L_{(+)}|l,m\rangle]$

$= L_+[L^2|l,m\rangle]$

$= L_+[l(l+1)\hbar^2 |l,m\rangle]$

$= l(l+1)\hbar^2 [L_{(+)}|l,m\rangle]$

This shows that $[L_{(+)}|l,m\rangle]$ is an eigen state of L^2 with eigenvalue $l(l+1)\hbar^2$

⊙ Hence $[L_+|l,m\rangle]$ is eigen state of L_z with eigen value of $(m_l+1)\hbar$. But for operator L_z, eigen state corresponding to eigen value $(m_l+1)\hbar$ is $|l, m+1\rangle$.

Hence job of $L_{(+)}$ Operator is to raise the [redacted] state of eigenfunction for which eigenvalue is raised by 1. [redacted].

Similarly job of L_- operator is to drop the eigen value by 1 to lower level.

$$\boxed{L_z[L_{(-)}|l,m\rangle] = \hbar(m_l-1)[L_{(-)}|l,m\rangle]}$$

★ From these two, it means $L_{(+)}$ raises $|l,m\rangle$ to $|l,m+1\rangle$

⇓

$L_{(+)}|l,m\rangle = c_1|l,m+1\rangle$

Also, $[L^2, L_z] \;|\; L_+|l,m\rangle = 0$

Note that Now since states as changes, it is not eigen value problem →

$$\boxed{\begin{aligned} L_{(+)}|l,m\rangle &= c_1 |l, m+1\rangle \\ L_{(-)}|l,m\rangle &= c_2 |l, m-1\rangle \end{aligned}}$$

i.e. let C_1, C_2 be [redacted] constant associated with $L_{(+)}$ & $L_{(-)}$ operators respectively.

$$\Rightarrow \left\langle L_{(+)} |l,m\rangle \middle| L_{(+)} |l,m\rangle \right\rangle = |C_1|^2 \quad \text{— (1)}$$

$$\left\langle L_{(-)} |l,m\rangle \middle| L_{(-)} |l,m\rangle \right\rangle = |C_2|^2 \quad \text{— (2)}$$

this is because $|l,m\rangle$ & $|l,m+1\rangle$ are orthonormal vectors !!

From (1), $\langle l,m | L_{(-)} L_{(+)} |l,m\rangle = |C_1|^2$ — (3)

(using the property of Hermitian adjoints)

$L_{(+)}$ and $L_{(-)}$ are adjoints

Similarly From (2)

$$\langle l,m | L_{(+)} L_{(-)} |l,m\rangle = |C_2|^2 \quad \text{— (4)}$$

From (3) & (4)

$$\Rightarrow \begin{cases} |C_1|^2 \Leftrightarrow \text{expectation value of } L_{(-)} L_{(+)} \\ |C_2|^2 \Leftrightarrow \text{expectation value of } L_{(+)} L_{(-)} \end{cases}$$

actually in these 2 RHS has no 'real' meaning !!

Now we can write,

$$L_- L_+ = (L_x - iL_y)(L_x + iL_y)$$

$$= L_x^2 + i(L_x L_y - L_y L_x) + L_y^2$$

$$= L^2 - L_z^2 + i[L_x L_y]$$

$$= L^2 - L_z^2 + i\, i\hbar L_z$$

$$= L^2 - L_z^2 - \hbar L_z$$

(*) $\langle l,m | L_z^2 | l,m\rangle$

$\Leftrightarrow \langle \psi(l,m) | L_z^2 \psi(l,m)\rangle$

$\Leftrightarrow \langle \psi(l,m) | L_z L_z \psi(l,m)\rangle$

$\Leftrightarrow \langle \psi(l,m) | L_z m\hbar \psi(l,m)\rangle$

$\Leftrightarrow (m\hbar) \langle \psi(l,m) | L_z \psi(l,m)\rangle$

$\Leftrightarrow (m\hbar)^2 \langle \psi(l,m) | \psi(l,m)\rangle = (m\hbar)^2$

Putting it in (3),

$$\langle l,m | L^2 - L_z^2 - \hbar L_z | l,m\rangle = |C_1|$$

$$|C_1|^2 = \langle l,m | L^2 | l,m\rangle - \underbrace{\langle l,m | L_z^2 | l,m\rangle} - \hbar \langle l,m | L_z | l,m\rangle$$

$$= l(l+1)\hbar^2 - m^2\hbar^2 - m\hbar^2$$

$$\Rightarrow |C_1|^2 = [l(l+1) - m(m+1)]\hbar^2$$

$$\Rightarrow |C_1|^2 = [(l^2-m^2)+(l-m)]\hbar^2$$

$$\boxed{|C_1|^2 = [(l-m)\ (l+m+1)]\hbar^2}$$

We are give Y_3^0 ($0 \leftarrow m$, $3 \leftarrow l$)

we can calculate, Y_3^1, Y_3^{-1}, Y_3^2, Y_3^{-2}, ...

$$\boxed{\begin{aligned} &\checkmark\ L_{(+)}|l,m\rangle = \sqrt{(l-m)(l+m+1)}\ \hbar\ |l, m+1\rangle \\ &\checkmark\ L_{(-)}|l,m\rangle = \sqrt{(l+m)\ (l-m+1)}\ \hbar\ |l, m-1\rangle \end{aligned}}$$

From these 2 its clear that $L_{(+)}|2,2\rangle = 0$

$L_{(-)}|2,-2\rangle = 0$

If I require, L_x or L_y anywhere

$$L_{(+)} = L_x + iL_y$$

$$L_{(-)} = L_x - iL_y$$

$$\Rightarrow \boxed{L_x = \frac{L_{(+)} + L_{(-)}}{2}} \quad ; \quad \boxed{L_y = \frac{L_{(+)} - L_{(-)}}{2i}}$$

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,

Q) $Y_2^1 = \frac{1}{\sqrt{15}} \cos^2\theta \, e^{i\phi}$ (given)

find ΔL_x.

We are give $l = 2$ ✓
$m = 1$ ✓

$\Rightarrow Y_2^1 = |2,1\rangle$

$$\langle L_x \rangle = \langle 2,1| \frac{L_{(+)} + L_{(-)}}{2} | 2,1\rangle$$

$$= \frac{1}{2} \langle 2,1| L_{(+)} |2,1\rangle + \frac{1}{2} \langle 2,1| L_{(-)} |2,1\rangle$$

$$L_{(+)} |2,1\rangle = \sqrt{(2-1)(2+1+1)} \, \hbar \, |2,2\rangle$$

Now $|2,1\rangle$ and $|2,2\rangle$ are orthogonal
Hence upon multiplying, it gives 0.

$\Rightarrow \langle L_x \rangle = 0$

$$\langle L_x^2 \rangle = \frac{1}{4} \langle 2,1| \underbrace{L_{(+)}^2}_{} + \underbrace{L_{(-)}^2}_{} + L_+L_- + L_-L_+ |2,1\rangle$$

it will give 0

$$\Rightarrow \langle L_x^2 \rangle = \frac{1}{4} \langle 2,1| L_{(+)} L_{(-)} |2,1\rangle + \frac{1}{4} \langle 2,1| L_{(-)} L_{(+)} |2,1\rangle$$

$\Rightarrow$ first applying $L_{(-)}$, we get from 1^{st} term

$\frac{1}{4}\langle 2,1|\ L_+\ \sqrt{6}\hbar|\ 2,0\rangle$ [do not forget $\sqrt{\ }$]

[do not forget $\hbar$]

$= \frac{\sqrt{6}\hbar}{4}\langle 2,1|\ L_+\ |2,0\rangle$

$= \frac{\sqrt{6}}{4}\cdot \langle 2,1|\ \sqrt{6}\hbar|2,1\rangle$

$= \frac{6\hbar^2}{4}\cdot\langle 2,1||2,1\rangle$

$= \left(\frac{6\hbar^2}{4}\right)$

Similarly,

$\frac{1}{4}\langle 2,1|\ L_{(-)}\ L_{(+)}\ |2,1\rangle$

$= \frac{1}{4}\ \langle 2,1|\ L_{(-)}\ 2\hbar\ |2,2\rangle$

$= \frac{1}{4}\cdot 2\hbar\ \ \langle 2,1|\ 2\hbar\ |2,1\rangle$

$\hbar^2$

$\Rightarrow \langle L_x^2\rangle = \frac{5}{2}\hbar^2$

$\Rightarrow \Delta L_x = \sqrt{\frac{5}{2}}\hbar$

Hence, just with knowledge of Quantum Numbers (m,l) we have calculated $\langle L_x\rangle, \langle L_x^2\rangle$ & $\langle L_y\rangle, \langle L_y^2\rangle$

Coming to Orbitals,

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 !!

$s = \left(\frac{1}{2}\right)$

$m_s = -s$ to $+s$ $(2s+1$ values$)$ $[-s, -s+1, \ldots\ldots s-1, s]$

$= \pm\left(\frac{1}{2}\right)$

$$\left.\begin{array}{l} S_z|s,m\rangle = \pm\frac{1}{2}\hbar|s,m\rangle \\ S_y|s,m\rangle = \pm\frac{1}{2}\hbar|s,m\rangle \\ S_x|s,m\rangle = \pm\frac{1}{2}\hbar|s,m\rangle \end{array}\right\}$$

?? can be in any direction

We have all similar results,

$$S_{(+)} = [S_x + iS_y] \qquad S_{(+)}|s,m\rangle = \sqrt{(s-m)(s+m+1)}\,\hbar|s,m+1\rangle$$

$$S_{(-)} = [S_x - iS_y] \qquad S_{(-)}|s,m\rangle = \sqrt{(s+m)(s-m+1)}\,\hbar|s,m-1\rangle$$

→ 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 there. And corresponding n orthogonal eigenfunctions $|\phi_i\rangle_s$

SPIN $\frac{1}{2}$ PROBLEM

⇒ for $s = \left(\frac{1}{2}\right)$

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 $S_x = \pm \frac{1}{2}\hbar$

σ_x is 2×2 matrix whose eigen value is ± 1

$$E.V.(\sigma_x) = \pm 1$$

$$\Rightarrow \boxed{S_x = \frac{1}{2}\hbar \, \sigma_x}$$

operator in matrix form

similarly,

$$\boxed{S_y = \frac{1}{2}\hbar \, \sigma_y}$$

$$\boxed{S_z = \frac{1}{2}\hbar \, \sigma_z}$$

$$\left.\begin{aligned} E.V.(\sigma_y) &= \pm 1 \\ E.V.(\sigma_z) &= \pm 1 \end{aligned}\right\}$$

2×2 matrices with eigen value is ±1

$$S^2 = S_x^2 + S_y^2 + S_z^2$$

$$= \frac{3}{4}\hbar^2$$

$$= s(s+1)\hbar^2$$

$$\neq S^2$$

$$\left.\begin{aligned} S_x \psi_1 &= \tfrac{1}{2}\hbar\, \psi_1 \\ S_x \psi_2 &\;\; -\tfrac{1}{2}\hbar\, \psi_2 \end{aligned}\right\}$$ upon measurement, we can have 2 values.

$l \qquad m_l$

i.e. $$S_x \left| \tfrac{1}{2}, \tfrac{1}{2} \right\rangle = \left(\tfrac{1}{2}\right)\hbar \left| \tfrac{1}{2}, \tfrac{1}{2} \right\rangle$$

$$S_x \left| \tfrac{1}{2}, -\tfrac{1}{2} \right\rangle = \left(-\tfrac{1}{2}\right)\hbar \left| \tfrac{1}{2}, -\tfrac{1}{2} \right\rangle$$

we write $\left| \tfrac{1}{2}, \tfrac{1}{2} \right\rangle$ as χ_+ : spin up state ↑
or
spin up vector

$\left| \tfrac{1}{2}, -\tfrac{1}{2} \right\rangle$ as χ_- : spin down state ↓
or
spin down vector

Now we can write,

$$\boxed{\begin{aligned} S_x \chi_{(+)} &= \tfrac{1}{2}\hbar\, \chi_{(+)} \\ S_x \chi_{(-)} &= -\tfrac{1}{2}\hbar\, \chi_{(-)} \end{aligned}}$$ ⟸ $\left(\tfrac{1}{2}\right)$ spin Eigen Value Problem

state of any $\tfrac{1}{2}$ spin particle

$$|\chi\rangle = c_1 |\chi_{(+)}\rangle + c_2 |\chi_{(-)}\rangle$$

upon normalization

$$\langle \chi | \chi \rangle = 1 \quad \Rightarrow \quad c_1^2 + c_2^2 = 1$$

★ $$\underset{(2\times 2)}{S_x}\ \underset{(2\times 1)}{\chi_{(+)}} = \frac{1}{2}\hbar\,[\chi_{(+)}]_{2\times 1}$$ ⟸ Matrix Representation

Hence state is a ~~...~~ column matrix

Orthonormal vectors

$$|\chi\rangle = \begin{bmatrix} c_1 \\ c_2 \end{bmatrix} = c_1\begin{bmatrix} 1 \\ 0 \end{bmatrix} + c_2\begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

(★) In general $\psi = c_1\phi_1 + c_2\phi_2 + c_3\phi_3 \ldots = c_1\begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix} + c_2\begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix} + \ldots$

ψ (state function), ϕ_1, ϕ_2 (orthogonal eigen function)

$|\chi_{(+)}\rangle = |\frac{1}{2}, \frac{1}{2}\rangle =$ Matrix Representation $\begin{bmatrix} 1 \\ 0 \end{bmatrix}$

$|\chi_{(-)}\rangle = |\frac{1}{2}, -\frac{1}{2}\rangle =$ Matrix Representation $\begin{bmatrix} 0 \\ 1 \end{bmatrix}$

Also note, orthogonality,
$\langle \chi_{(+)} | \chi_{(-)} \rangle =$ $\begin{bmatrix} 1 & 0 \end{bmatrix}\begin{bmatrix} 0 \\ 1 \end{bmatrix} = [0]$

1 | Tut 3

(1) (i) only function of r
no dependence on θ and ϕ
$\Rightarrow l = 0$

(ii) $\vec{S} \times \vec{S} = i\hbar\,\vec{S}$

$[S^2, S_x] = 0$

$S_x S_y + S_y S_x = 0$: Anti Commutation

or

$\sigma_x\sigma_y + \sigma_y\sigma_x = 0$

(2) $S^2 = \frac{3}{4}\hbar^2$

16 $\chi = A\begin{pmatrix} 3i \\ 4 \end{pmatrix}$

$\langle \chi | \chi \rangle = 1$

$\left.\langle \chi | = A^* \begin{bmatrix} -3i & 4 \end{bmatrix} \right\}$ ✪

$\langle \chi | \chi \rangle = |A^*|^2 \begin{bmatrix} -3i & 4 \end{bmatrix} \begin{bmatrix} 3i \\ 4 \end{bmatrix} = |A|^2 (9+16) = 1$

$\Rightarrow \quad \underline{\underline{|A| = \frac{1}{5}}}$

$\Rightarrow \quad \chi = \frac{1}{5}\begin{bmatrix} 3i \\ 4 \end{bmatrix}$

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,
$\langle S_x \rangle = \langle \chi | S_x | \chi \rangle$ $\qquad \langle S_x^2 \rangle = \langle \chi | S_x^2 | \chi \rangle$

But what is S_x??

$\underbrace{S_x = \frac{1}{2}\hbar\sigma_x}_{\text{matrix form}}$ & $\underbrace{S_x = \frac{S_{(+)} + S_{(-)}}{2}}_{\text{relation to ladder operators.}}$ We know

$$S_x = \begin{bmatrix} \langle \chi_+ | S_x | \chi_+ \rangle & \langle \chi_+ | S_x | \chi_- \rangle \\ \langle \chi_- | S_x | \chi_+ \rangle & \langle \chi_- | S_x | \chi_- \rangle \end{bmatrix}$$

← refer [9.5] H.C. Verma for its derivation P: 264

or

refer to end of this lecture !!

$$= \frac{1}{2}\begin{bmatrix} \langle \chi_+ | S_{(+)} + S_{(-)} | \chi_+ \rangle & \dots \\ \dots & \dots \end{bmatrix}$$

$\langle \chi_+ | S_+ | \chi_+ \rangle + \langle \chi_+ | S_- | \chi_- \rangle$

Note that $S_{(+)}\chi_+ = 0 \qquad S_{(-)}\chi_{(-)} = 0$

$S_{(+)}\chi_{(-)} = \sqrt{\left(\frac{1}{2} + \left(\frac{1}{2}\right)\right)\left(\frac{1}{2} - \frac{1}{2} + 1\right)}\,\hbar = \hbar\,\chi_{(+)}$ ✓

i.e.

$$\boxed{\begin{aligned} S_{(+)}\, \chi_{(-)} &= \hbar\, \chi_{(+)} \\ S_{(-)}\, \chi_{(+)} &= \hbar\, \chi_{(-)} \end{aligned}} \qquad \boxed{\begin{aligned} S_{(+)}\, \chi_{(+)} &= 0 \\ S_{(-)}\, \chi_{(-)} &= 0 \end{aligned}}$$

$$\Rightarrow S_x = \frac{1}{2}\begin{bmatrix} 0 & \hbar \\ \hbar & 0 \end{bmatrix} = \frac{1}{2}\hbar \underbrace{\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}}_{[\sigma_x]}$$

$$\boxed{\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}}$$

Now $S_y = \dfrac{1}{2i}\begin{bmatrix} \langle \chi_+ | S_{(+)} - S_{(-)} | \chi_- \rangle & \cdots \\ \cdots & \cdots \end{bmatrix}$

$$= \frac{1}{2i}\begin{bmatrix} 0 & \hbar \\ -\hbar & 0 \end{bmatrix}$$

$$= \frac{1}{2}\hbar \underbrace{\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}}_{[\sigma_y]}$$

$$\boxed{\sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}}$$

L_x and L_y from knowledge 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.

$$i\hbar S_z = S_x S_y - S_y S_x$$

$$\underline{\underline{S_x S_y - S_y S_x = i\hbar S_z}} \quad — (1)$$

$$\Rightarrow \quad S_z = \frac{1}{2}\hbar\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix} \qquad \boxed{\sigma_z = \begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}}$$

To prove

$$\underline{\underline{S_x S_y + S_y S_x = 0}} \quad — (2)$$

$$\frac{1}{i\hbar}\left[i\hbar S_x S_y + i\hbar S_y S_x \right] \qquad \text{[multiply \& divide by } i\hbar\text{]}$$

$$= \frac{1}{i\hbar}\left[S_x [S_z, S_x] + [S_z, S_x] S_x \right]$$

$$= \frac{1}{i\hbar}\left[\cancel{S_x S_z S_x} - S_x^2 S_z + S_z S_x^2 - \cancel{S_x S_z S_x} \right]$$

Use $S_x^2 = I$, $S_y^2 = I$

$$= 0$$

$$\underbrace{\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}}\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix} - \begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}\underbrace{\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}}$$

$$= \begin{bmatrix}0 & 1\\ -1 & 0\end{bmatrix}\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix} - \begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}\begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}$$

$$= \begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix} - \begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix} = \underline{0}$$

$$\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix}\begin{bmatrix}0 & 1\\ 1 & 0\end{bmatrix} = \begin{bmatrix}1 & 0\\ 0 & 1\end{bmatrix}$$

From (1) and (2),

$$\boxed{S_x S_y + S_y S_x = 0}$$

$$\underline{S_x S_y - S_y S_x = i\hbar S_z}$$

$$S_x S_y + S_x S_y = i\hbar S_z$$

$$\Rightarrow \boxed{S_x S_y = \frac{i\hbar S_z}{2}}$$

$$\Rightarrow \frac{1}{2\cdot 2}\hbar^2 \sigma_x \sigma_y = \frac{i\hbar}{2} S_z = \frac{i\hbar}{2}\frac{\hbar}{2}\sigma_z$$

$$\Rightarrow \boxed{\sigma_x \sigma_y = i\sigma_z}$$

$$\boxed{\sigma_x \sigma_y \sigma_z = i[I]_{2\times 2}}$$

$$\sigma_z = \begin{bmatrix}1 & 0\\ 0 & -1\end{bmatrix}$$

To determine eigen values of matrix

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

$$|\sigma_x - \lambda_x I| = 0$$

$$\Rightarrow \begin{vmatrix} -\lambda_x & 1 \\ 1 & -\lambda_x \end{vmatrix} = 0$$

$$\Rightarrow \lambda_x^2 - 1 = 0$$

$$\Rightarrow \underline{\underline{\lambda_x = \pm 1}}$$

$$\sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$$

$$|\sigma_y - \lambda_y I| = 0$$

$$\Rightarrow \begin{vmatrix} -\lambda_y & -i \\ i & -\lambda_y \end{vmatrix} = 0$$

$$\Rightarrow \lambda_y^2 - 1 = 0$$

$$\Rightarrow \underline{\underline{\lambda_y = \pm 1}}$$

$$\sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

$$|\sigma_z - \lambda_z I| = 0$$

$$\Rightarrow \begin{vmatrix} 1-\lambda_z & 0 \\ 0 & (-1-\lambda_z) \end{vmatrix} = 0$$

$$\Rightarrow (1-\lambda_z)(1+\lambda_z) = 0$$

$$\Rightarrow \lambda_z^2 = 1$$

$$\Rightarrow \underline{\underline{\lambda_z = \pm 1}}$$

~~Trace = Sum of diagonals = 0~~ for S_x, S_y, S_z

Coming back to Q-16)

$$\langle \chi | S_x | \chi \rangle = \langle \chi | S_x \chi \rangle = [\bar{X}]^T [S_x][X]$$

$$= \begin{bmatrix} -3i & 4 \end{bmatrix} \left| \frac{1}{2}\hbar \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \right| \begin{bmatrix} 3i \\ 4 \end{bmatrix}$$

$$= \frac{1}{2}\hbar \begin{bmatrix} 4 & -3i \end{bmatrix} \begin{bmatrix} 3i \\ 4 \end{bmatrix}$$

Note that matrix multiplication is associative....

$$= \frac{1}{2}\hbar \cdot 0 = 0$$

$$\langle \chi | S_x^2 | \chi \rangle$$

$$= \begin{bmatrix} -3i & 4 \end{bmatrix} \frac{1}{2^2}\hbar^2 \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 3i \\ 4 \end{bmatrix}$$

$$= \frac{25}{4}\hbar^2$$

$$\Rightarrow \Delta S_x = \sqrt{\frac{25}{4}\hbar^2} = \underline{\underline{\frac{5}{2}\hbar}}$$

(17) $(5,5,4) \Rightarrow g_1 = 3$
$(8,1,1) \Rightarrow g_2 = 3$
$(7,4,1) \quad g_3 = 6$

} Spin is not considered.

⊙ General Wave Function of Spin be

$$\chi = \alpha \chi_{(+)} + \beta \chi_{(-)}$$

We can write χ as $\begin{bmatrix} \alpha \\ \beta \end{bmatrix}$ with $\underbrace{\chi_{(+)} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \ \& \ \chi_{(-)} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}}_{\text{Basis vectors}}$

Let us take general operator S

$$S(\chi) = \alpha\, S(\chi_{(+)}) + \beta\, S(\chi_{(-)})$$
$$= \alpha\, \underline{c_1\, \chi_{(+)}} + \beta\, \underline{c_2\, \chi_{(-)}} \quad (\text{say})$$
$$= \alpha' \chi_{(+)} + \beta' \chi_{(-)}$$
$$= \chi' \quad (\text{say})$$

Now we can write χ' as $\begin{bmatrix} \alpha' \\ \beta' \end{bmatrix}$

What are α' and β'

$\underline{\alpha'} = \langle \chi_{(+)} | \chi' \rangle \quad \& \quad \beta = \langle \chi_{(-)} | \chi' \rangle$

$$= \langle \chi_{(+)} | \alpha S(\chi_{(+)}) + \beta S(\chi_{(-)}) \rangle$$
$$= \alpha \langle \chi_{(+)} | S(\chi_{(+)}) \rangle + \beta \langle \chi_{(+)} | S(\chi_{(-)}) \rangle$$
$$= \underline{\alpha \langle \chi_{(+)} | S | \chi_{(+)} \rangle + \beta \langle \chi_{(+)} | S | \chi_{(-)} \rangle}$$

Similarly

$$\underline{\beta'} = \langle \chi_{(-)} | \chi' \rangle = \langle \chi_{(-)} | \alpha S(\chi_{(+)}) + \beta S(\chi_{(-)}) \rangle$$
$$= \underline{\alpha \langle \chi_{(-)} | S | \chi_{(+)} \rangle + \beta \langle \chi_{(-)} | S | \chi_{(+)} \rangle}$$

Now $\chi' = \begin{bmatrix} \alpha \\ \beta \end{bmatrix}$

$$= \begin{bmatrix} \alpha \langle \chi_{(+)} | S | \chi_{(+)} \rangle + \beta \langle \chi_{(+)} | S | \chi_{(-)} \rangle \\ \alpha \langle \chi_{(-)} | S | \chi_{(+)} \rangle + \beta \langle \chi_{(-)} | S | \chi_{(-)} \rangle \end{bmatrix}$$

$$= \begin{bmatrix} \langle \chi_{(+)} | S | \chi_{(+)} \rangle & \langle \chi_{(+)} | S | \chi_{(-)} \rangle \\ \langle \chi_{(-)} | S | \chi_{(+)} \rangle & \langle \chi_{(-)} | S | \chi_{(-)} \rangle \end{bmatrix} \begin{bmatrix} \alpha \\ \beta \end{bmatrix}$$

$$= S \begin{bmatrix} \alpha \\ \beta \end{bmatrix}$$

$$\Rightarrow \quad \boxed{S = \begin{bmatrix} \langle \chi_{(+)} | S | \chi_{(+)} \rangle & \langle \chi_{(+)} | S | \chi_{(-)} \rangle \\ \langle \chi_{(-)} | S | \chi_{(+)} \rangle & \langle \chi_{(-)} | S | \chi_{(-)} \rangle \end{bmatrix}}$$

Note that I can write

- $\vec{\sigma} = \sigma_x \hat{i} + \sigma_y \hat{j} + \sigma_z \hat{k}$

$$\vec{S} = \frac{1}{2}\hbar \vec{\sigma} = \frac{1}{2}\hbar \sigma_x \hat{i} + \frac{1}{2}\hbar \sigma_y \hat{j} + \frac{1}{2}\hbar \sigma_z \hat{k}$$

$$= S_x \hat{i} + S_y \hat{j} + S_z \hat{k}$$

- Also $\boxed{\vec{\sigma} \times \vec{\sigma} = 2i\vec{\sigma}}$

---

1. Anti commutation
2. $\sigma_x \sigma_y - \sigma_y \sigma_x = 2i\sigma_z$
3. $\det(\sigma_i) = -1$
4. $\sigma_i^2 = I$
5. $\sigma_x \sigma_y \sigma_z = iI$
6. $\text{Trace}(\sigma_i) = 0$

<u>Properties of Pauli matrices</u>

→ Since eigen values of S_x, S_y, S_z are $\frac{1}{2}\hbar$ ⇒ Angular Momentum of Spin in any direction can take $\left(\frac{\hbar}{2}\right)$ value and $|S| = \sqrt{\frac{3\hbar^2}{4}}$

So Basically, let the wave function be

$$|\psi\rangle = \sum c_i |\phi_i\rangle \qquad \text{eg. } \begin{bmatrix} c_1 \\ c_2 \\ c_3 \end{bmatrix}$$

Now applying an operator A upon $|\psi\rangle$, whose eigen function are $|\phi_i\rangle$'s

$$A|\psi\rangle = \sum c_i A|\phi_i\rangle$$

$$= \sum c_i \lambda_i |\phi_i\rangle$$

$$= \sum \lambda_i' |\phi_i\rangle$$

Hence, new matrix is $\begin{bmatrix} \lambda_1 \\ \lambda_2 \\ \lambda_3 \end{bmatrix}$

Now,

$$\lambda_i' = \langle \phi_i | A|\psi\rangle$$

$$= \langle \phi_i | \sum_j c_j A|\phi_j\rangle$$

$$= \sum_j c_j \langle \phi_i | A | \phi_j\rangle$$

Now this is a matrix representation,

$$\begin{bmatrix} \lambda_1 \\ \lambda_2 \\ \lambda_3 \end{bmatrix} = \begin{bmatrix} \langle\phi_1|A|\phi_1\rangle & \langle\phi_1|A|\phi_2\rangle & \langle\phi_1|A|\phi_3\rangle \\ \langle\phi_2|A|\phi_1\rangle & \langle\phi_2|A|\phi_1\rangle & \langle\phi_2|A|\phi_3\rangle \\ \langle\phi_3|A|\phi_1\rangle & \langle\phi_3|A|\phi_2\rangle & \langle\phi_3|A|\phi_3\rangle \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ c_3 \end{bmatrix}$$

Quantum Physics (12)

Free e^- theory of metals

We have done

density of state, $g(\epsilon) = \dfrac{dN(\epsilon)}{d\epsilon}$

$$\Rightarrow \quad dN(\epsilon) = g(\epsilon)\, d\epsilon$$

$$N(\epsilon) = \int dN(\epsilon) = \int_0^{\epsilon} g(\epsilon)\, d\epsilon$$

Total no. of states = Total no. of states

For fermions, due to spin, 2 particles per state

if $s = \left(\frac{1}{2}\right)$

$$\Rightarrow N = 2 \int_0^{\epsilon_{f_0}} \underbrace{g(\epsilon)}_{\text{no. of cells}}\ \underbrace{f(\epsilon)}_{\text{no. of particles per cell}}\, d\epsilon$$

Total no. of particles

(*) There is a difference in the 2 'N's. Hence the factor of $f(\epsilon)$.

$$g(\epsilon) = \frac{2\pi V}{h^3} (2m)^{\frac{3}{2}} \epsilon^{1/2} \checkmark$$

@ $T = 0$, $f(\epsilon) = 1$ for $\epsilon < \epsilon_{f_0}$

$$N = 2 \int_0^{\epsilon_{f_0}} 1 \cdot \frac{2\pi V}{h^3} (2m)^{\frac{3}{2}} \epsilon^{\frac{1}{2}} d\epsilon$$

$$\Rightarrow N = \frac{4\pi V}{h^3} (2m)^{\frac{3}{2}} \epsilon_f^{\frac{3}{2}} \frac{2}{3}$$

$$\boxed{\epsilon_{f_0} = \frac{\hbar^2}{2m} (3\pi^2 n)^{2/3}}$$

Total energy $E = \epsilon\, dN$

$$\Rightarrow E_T = \frac{4\pi V}{h^3} (2m)^{\frac{3}{2}} \int_0^{\epsilon_{f_0}} \epsilon^{\frac{3}{2}} d\epsilon = \frac{3}{2} N \epsilon_f^{-\frac{3}{2}} \frac{\epsilon^{\frac{5}{2}}}{\frac{5}{2}}$$

$$\Rightarrow \boxed{E_T = \frac{3}{5} N \epsilon_{f_0}}$$

We have calculated $g(\epsilon)\,d\epsilon$ as

$$\boxed{g(p)\,dp = \frac{d^3r\, d^3p}{h^3}}$$

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. (also called free electron)

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 space of motion of free electrons as cubical box.

For their motion, $H\psi = E\psi$

In cubical box, we know

$$\boxed{E = (n_x^2 + n_y^2 + n_z^2)\frac{h^2}{8mL^2}}$$

Now $n_x^2 + n_y^2 + n_z^2 = \left(\frac{8mL^2}{h^2}E\right) = R^2$ (say)

dN = No. of energy states between E and $E + dE$

= No. of states between $(n_x + dn_x)$, $(n_y + dn_y)$, $(n_z + dn_z)$

$$= \frac{1}{8} \cdot 4\pi R^2\, dR$$

$$= \frac{1}{8} \cdot 4\pi \frac{8mL^2}{h^2} E \cdot \sqrt{\frac{8mL^2}{h^2}}\, \frac{1}{2} \frac{dE}{\sqrt{E}}$$

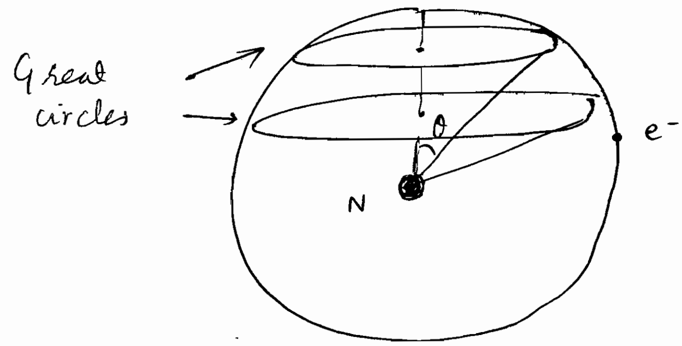
$$dN = \frac{2\pi V}{h^3} (2m)^{\frac{3}{2}} E^{\frac{1}{2}}\, dE$$

$$\Rightarrow \boxed{g(\epsilon)\, d\epsilon = \frac{2\pi V}{h^3} (2m)^{\frac{3}{2}} E^{\frac{1}{2}}}$$

⊙ 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.



$\forall r,\ 0 < \theta < \pi$

$\forall \theta,\ 0 < \phi < 2\pi$

$\forall \theta$: we have 1 great circle

$\forall \theta$: 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

$$\Rightarrow \mu = \frac{m_p m_e}{m_p + m_e} = \frac{m_e}{1 + \frac{m_e}{m_p}} \simeq m_e$$

Similarly Centre of Mass corresponds to center of nucleus.

$$H = \frac{p^2}{2\mu} + V = \frac{-\hbar^2}{2m_e} \nabla^2 + V(r)$$

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

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

$$\Rightarrow \nabla^2\psi + \frac{2\mu}{\hbar^2}(E-V)\psi = 0$$

Now,

$$\nabla^2\psi = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial\psi}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\left(\frac{\partial^2\psi}{\partial\phi^2}\right)$$

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

$$\Rightarrow \Theta\,\Phi\,\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial R}{\partial r}\right) + \frac{R\,\Phi}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left[\sin\theta\frac{\partial\Theta}{\partial\theta}\right]$$

$$+ \frac{R\,\Theta}{r^2\sin^2\theta}\left(\frac{\partial^2\Phi}{\partial\phi^2}\right) + \frac{2\mu}{\hbar^2}(E-V)\,R\,\Theta\,\Phi = 0$$

$\Rightarrow$ Multiply by $\dfrac{r^2\sin^2\theta}{R\,\Theta\,\Phi}$

$$\Rightarrow \frac{\sin^2\theta}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{\sin\theta}{\Theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)$$

$$+ \underbrace{\frac{1}{\Phi}\left(\frac{\partial^2\Phi}{\partial\phi^2}\right)}_{\text{separate it out by taking it on RHS}} + \frac{2\mu r^2\sin^2\theta}{\hbar^2}(E-V) = 0$$

$$\Rightarrow \frac{\sin^2\theta}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{2\mu r^2\sin^2\theta}{\hbar^2}(E-V) = m^2 - \frac{\sin\theta}{\Theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)$$

dividing by $\sin^2\theta$

$$\Rightarrow \frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{2\mu r^2}{\hbar^2}(E-V) = \frac{m^2}{\sin^2\theta} - \frac{1}{\Theta\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)$$

$$f_1(r) = f_2(\theta) = \lambda \text{ (say)}$$

$$\Rightarrow \frac{m^2}{\sin^2\theta} - \frac{1}{\Theta \sin\theta} \frac{d}{d\theta}\left(\sin\theta \frac{d\Theta}{d\theta}\right) = \lambda$$

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.

Solutions are : $\lambda = l(l+1)$

$|m| < l$

$\Theta = B P_l^m(\cos\theta)$

where $P_l^m(x)$ are associated Legendre's Polynomials

We have already solved,

$$\Phi = A e^{im\phi}$$

$$\Rightarrow \boxed{\psi(r,\theta,\phi) = R(r)\, Y_l^{m_l}(\theta,\phi)} \Leftarrow$$

Till this point solution is same as for Angular Momentum

Motion ϕ fixes m_l : and gives L_z

Motion w.r.t. θ fixes l : and gives $|\vec{L}| = \sqrt{l(l+1)}$

Motion w.r.t. r fixes 'n' : and gives E

Now our aim is to obtain $R(r)$

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

$$\Rightarrow \frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \frac{2\mu r^2}{\hbar^2}\left[E - V - \frac{\ell(\ell+1)\hbar^2}{2\mu r^2}\right]R = 0$$

Eqn 20.3. of Verma

Let $V_{eff} = V + \underbrace{\frac{\ell(\ell+1)\hbar^2}{2\mu r^2}}$

$\uparrow$
Centrifugal distortion

Let $\dfrac{R(r)}{} = \left(\dfrac{u(r)}{r}\right)$ And put $\rho(r) = kr$

$$\Rightarrow \frac{1}{r}\frac{d^2u}{dr^2} + \frac{2\mu r^2}{\hbar^2}(E - V_{eff})\, u_r = 0$$

Solutions of this differential equation are

$$\frac{d^2u}{d\rho^2} = k^2\rho \qquad u(\rho) = Ae^{k\rho} + Ae^{-kr}$$

as $r \to \infty$, $\rho \to \infty$ $\Rightarrow$ $u(\rho) = Ae^{-kr}$

For better solution, $u(r) = V(\rho)\; u(\rho)$

$$V(\rho) = \sum_{\ell=0}^{\infty} a_\ell \rho^\ell$$

Series will terminate at $n = j + l + 1$
where l is any integer.
j is any integer.

$$\boxed{n_{min} = 1}$$

$R(r) = R_n(r)$: Laguerre's Polynomials

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

Energy from Bohr

Substituting k,

$$\boxed{E_n = -\frac{\mu e^4}{8\epsilon_0^2 h^2}\frac{1}{n^2}} \boxed{= -\frac{13.6}{n^2}\,eV}$$

define $\boxed{R = \frac{\mu e^4}{8\epsilon_0^2 c h^3}}$ $\Rightarrow$ $\boxed{E_n = -\frac{Rhc}{n^2}}$

= Rydberg's const.

No. restriction on n $\Rightarrow$ $1 \leq n < \infty$

$$\Rightarrow \psi(r,\theta,\phi) = R_n^l \,\Theta_l^m \,\Phi^m$$
$$= R_n^l \, P_l^{m_l}(\cos\theta)\, e^{im\phi}$$

✔ $E_n = -\frac{Rhc}{n^2}$ where $R = \frac{\mu e^4}{8\epsilon_0^2 c h^3}$

$= 1.09 \times 10^7 \ m^{-1}$

$$= -\frac{13.6}{n^2}\ eV$$

Q6 $\boxed{\psi(n,l,m)}$

$$\psi_{n,l,m}(r,0) = \frac{1}{\sqrt{14}}\left[2\ \psi_{100}(r) - 3\ \psi_{200}(r) + \psi_{322}(r)\right]$$

(i) $P = \left(\frac{9}{14}\right)$ $\quad \langle \phi_i | \psi \rangle^2 = |c_i|^2$

(ii) $\langle H \rangle = \frac{4}{14} \langle 100 | H | 100 \rangle + \frac{9}{14} \langle 200 | H | 200 \rangle$

$+ \frac{1}{14} \langle 322 | H | 322 \rangle$

$= \frac{4}{14} \cdot \left(\frac{-13\cdot 6}{1}\right) + \frac{9}{14}\left(-\frac{13\cdot 6}{4}\right) + \frac{1}{14}\left(\frac{-13\cdot 6}{9}\right)$

$L_z = m_l \hbar$

$\langle L_z \rangle = \langle n,l,m | L_z | n,lm \rangle$

$= \frac{1}{14}\ 2\hbar = \left(\frac{\hbar}{7}\right)$

Q 4) $\quad P(r)\,dr = \psi^*(r)\ \psi(r)\ 4\pi r^2\,dr$

$\psi(r) = \frac{1}{\sqrt{\pi}\, a^{\frac{3}{2}}}\, e^{-\left(\frac{r}{a}\right)}$

$\int_0^{\infty} P_{(r)}\,dr = 1 \ \rightarrow\ \frac{4\pi}{\pi a^3}\int_0^{\infty} r^2 e^{-\left(\frac{r}{a}\right)}\,dr = 1$

$\int_0^{\infty} e^{-x} x^{n-1}\,dx = \Gamma n$ $\quad \Rightarrow \frac{4\pi}{\pi a^3}\, a^2 \cdot a \int_0^{\infty} x^2 e^{-x}\,dx$ $\quad$ Put $\left(\frac{r}{a}\right) = x$

$=$

$$P(r) = \frac{4\pi}{\pi a^3} e^{-\frac{2r}{a}} r^2$$

<u>Maximum</u> at $\left.\frac{dP(r)}{dr}\right|_{r=r_{min}} = 0$ $\left.\frac{d^2P(r)}{dr^2}\right|_{r=r_{min}} < 0$

$$\cancel{e^{-\frac{2r}{a}}}(2r) + r^2\left(\cancel{e^{-\frac{2r}{a}}}\right)\left(-\frac{2}{a}\right) = 0$$

$$\Rightarrow \boxed{r = a}$$ ✓

Also Note,

$\psi(100) = \psi(1s)$ ⊙ $n_{min} = 1$, $l_{min} = 0$

$\psi(200) = \psi(2s)$

$\psi(210) = \psi(2p_x)$

$\psi(211) = \psi(2p_y)$

$\psi(212) = \psi(2p_z)$

$(2, 8, 18, \ldots)$ ← remember shell configuration !!

⊙ For given n, there are n values of l, $[0, 1, 2, \ldots n-1]$

⊙ For each l, $(2l+1)$ values of m_l

⊙ Also for every m, 2 spin

$\Rightarrow$ For a given E_n, $\underline{2n^2}$ degenerate states $\left[2\sum_{0}^{n-1}(2l+1) = 2n^2\right]$

⊙ $n=1$: ground state

$$\boxed{\psi(1,0,0) = \frac{1}{\sqrt{\pi}\, a^{3/2}} e^{-\frac{r}{a}}}$$

$$\boxed{\begin{aligned} a &: \text{Bohr Radius} \\ &= \left(\frac{4\pi\varepsilon_0 \hbar^2}{m_e e^2}\right) \\ &= 0.53\,\mathring{A} \end{aligned}}$$

$$\langle r^n \rangle = \int_0^\infty \left(\frac{1}{\sqrt{\pi}a^{3/2}} e^{-\frac{r}{a}} \; r^n \; \frac{1}{\sqrt{\pi}a^{3/2}} e^{-\frac{r}{a}}\right) 4\pi r^2 \, dr$$

$$= \frac{4}{a^3}\int_0^\infty r^{n+2} e^{-\frac{2r}{a}} dr$$

$\frac{2r}{a} = x$

$$= \frac{4}{a^3}\left(\frac{a}{2}\right)^{n+3} \int_0^\infty x^{n+2} e^{-x} dx$$

$$= \frac{4}{a^3} \left(\frac{a}{2}\right)^{n+3} \Gamma{n+3}$$

$$\boxed{\langle r^n \rangle = \frac{1}{2}\left(\frac{a}{2}\right)^n \Gamma{n+3}}$$ in ground state $\psi(1,0,0)$

$$\langle r \rangle = \frac{1}{2} \frac{a}{2} \Gamma 4 = \frac{1}{4} a . \lfloor 3 = \left(\frac{3a}{2}\right)$$

$$\langle \frac{1}{r} \rangle = \frac{1}{2}\left(\frac{a}{2}\right)^{-1} \Gamma 2 = \left(\frac{1}{a}\right)$$

$\boxed{4\pi r^2 : \text{मत भूलना}}$

$$\langle r^2 \rangle = \frac{1}{2}\left(\frac{a}{2}\right)^2 \Gamma 5 = \frac{4.3.2.\ a^2}{8} = 3a^2$$

$$\langle r^n \rangle = \langle n, l, m \mid r^n \mid n, l, m \rangle$$

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

$$\langle V \rangle = \frac{-e^2}{4\pi\varepsilon_0} \langle \frac{1}{r} \rangle$$

$$\langle E \rangle = \langle n | H | n \rangle = -\frac{13.6}{n^2} \text{ eV}$$

$$\left[\langle T \rangle = \langle E \rangle - \langle V \rangle \right]$$

do not do by any other method

Quantum Mechanics (13)

19/02/2012

For any dynamical variable, rate of change of its expectation value is given by

$$\boxed{\frac{d}{dt}\langle a\rangle = \frac{1}{i\hbar}\langle [A, H]\rangle + \left\langle \frac{\partial A}{\partial t}\right\rangle}$$ Ehrenfest theorem

eg. (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 Ehrenfest Theorem

Description of motion of particle in quantum mechanics

From (1) $\frac{\partial}{\partial t}\langle x\rangle = \frac{1}{i\hbar}\langle [X, H]\rangle$

$$= \frac{1}{i\hbar}\left\langle \left[X, \frac{P_x^2}{2m} + V(x)\right]\right\rangle$$

$$= \frac{1}{i\hbar}\left\langle \left[X, \frac{P_x^2}{2m}\right]\right\rangle + \frac{1}{i\hbar}\langle [X, V_x]\rangle$$

$$= \frac{1}{i2m\hbar}\langle [X, P_x^2]\rangle$$

$$= \frac{1}{i2m\hbar}\, 2i\hbar P_x$$

$$= \left[\frac{\langle p_x\rangle}{m}\right]$$

$x\,(-i\hbar)^2 \frac{\partial^2}{\partial x^2}\psi$

$- (-i\hbar)^2 \frac{\partial^2}{\partial x^2}(x\psi)$

$= - (-i\hbar)^2 \frac{\partial^2}{}$

From ②,

$$\frac{\partial}{\partial t}\langle p_x\rangle = \frac{1}{i\hbar}\langle [P_x, H]\rangle$$

$$= \frac{1}{i\hbar}\langle [P_x, \frac{P_x^2}{2m}]\rangle + \frac{1}{i\hbar}\langle [P_x, V_x]\rangle$$

$$= \frac{1}{i\hbar}\langle [P_x, V_x]\rangle$$

$$= \frac{1}{i\hbar}\langle i\hbar\left(\frac{\partial V_{(x)}}{\partial x}\right)\rangle$$

$$= \langle -\frac{\partial V}{\partial x}\rangle$$

$$= -\langle \frac{\partial V}{\partial x}\rangle$$

$[P_x, V_x]\psi$

$-i\hbar\frac{\partial (V_x\psi)}{\partial x}$

$+ V_x\left(\cancel{i\hbar\frac{\partial}{\partial x}\psi}\right)$

$-\cancel{i\hbar V\frac{\partial}{\partial x}\psi} - i\hbar\psi\left(\frac{\partial V}{\partial x}\right)$

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

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' is a const. of motion eg. for free particle,

$$[p_x , H] = \left[p_x , \frac{p_x^2}{2m}\right] = 0$$

$\Rightarrow \langle p_x \rangle$ is a const. of motion.

$$\Rightarrow \frac{\partial \langle p_x \rangle}{\partial t} = \frac{1}{i\hbar}\langle [p_x, H]\rangle = 0 \;\Rightarrow\; \underline{\langle p_x \rangle = \text{const.}}$$

→ Prove that for a free particle momentum is a const. of motion.

Derivation of :→ $\displaystyle \frac{d}{dt}\langle a \rangle = \frac{1}{i\hbar}\langle [A,H]\rangle + \left\langle \frac{\partial A}{\partial t}\right\rangle$

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

$$\frac{d}{dt}\langle a \rangle = \left\langle \psi | A | \left(\frac{\partial \psi}{\partial t}\right) \right\rangle + \underbrace{\left\langle \psi \left| \frac{\partial A}{\partial t} \right| \psi \right\rangle}_{= \left\langle \frac{\partial A}{\partial t}\right\rangle} + \left\langle \frac{\partial \psi}{\partial t} | A | \psi \right\rangle$$

$$\Rightarrow \frac{d}{dt}\langle a \rangle = \left\langle \psi | A | \frac{\partial \psi}{\partial t} \right\rangle + \left\langle \frac{\partial \psi}{\partial t} | A | \psi \right\rangle + \left\langle \frac{\partial A}{\partial t}\right\rangle$$

$$H\psi = i\hbar \left(\frac{\partial \psi}{\partial t}\right) \quad \ldots$$

Time dependent Schrodinger wave Equation

$\boxed{\text{Note that time dependent Schrodinger Eqn is the only source of time derivatives of } \psi \text{ !!}}$

$$\Rightarrow \frac{d}{dt}\langle a \rangle = \frac{1}{i\hbar}\langle \psi | A | H\psi \rangle + \left\langle \frac{\partial \psi}{\partial t} | A | \psi \right\rangle$$

$$+\frac{1}{i\hbar} H\psi = \left(\frac{\partial \psi}{\partial t}\right) \Rightarrow \underbrace{\frac{-1}{i\hbar}\psi^* H}_{-\frac{1}{i\hbar}\langle \psi | H} = \frac{\partial \psi^*}{\partial t} = \left\langle \frac{\partial \psi}{\partial t}\right|$$

$$\Rightarrow \frac{d}{dt}\langle a \rangle = \frac{1}{i\hbar}\langle \psi | AH | \psi \rangle - \frac{1}{i\hbar}\langle \psi | HA | \psi \rangle$$

(using H is Hermitian)

$$\frac{d}{dt}\langle a\rangle = \frac{1}{i\hbar}\left[\langle\psi|AH|\psi\rangle - \langle\psi|HA|\psi\rangle\right] + \left\langle\frac{\partial A}{\partial t}\right\rangle$$

$$\boxed{\frac{\partial}{\partial t}\langle a\rangle = \frac{1}{i\hbar}\langle[A,H]\rangle + \left\langle\frac{\partial A}{\partial t}\right\rangle}$$

$$\star\ \boxed{\langle A\rangle \iff \langle\psi|A|\psi\rangle} \boxed{= \langle a\rangle}$$

Parabolic Potential Well (from advanced Quantum Mechanics)

We know

$$L_{(+)}|l,m\rangle = \sqrt{(l-m)(l+m+1)}\ \hbar\ |l,m+1\rangle$$

$$L_{(-)}|l,m\rangle = \sqrt{(l+m)(l-m+1)}\ \hbar\ |l,m-1\rangle$$

$$L_x = \frac{L_{(+)} + L_{(-)}}{2}$$

$$L_y = \frac{L_{(+)} - L_{(-)}}{2i}$$

From Harmonic Oscillator, we know

$$E_n = \left(n+\frac{1}{2}\right)\hbar\omega$$

$$\psi_n = C_n H_n(x)\, e^{-\frac{m\omega}{2\hbar}x^2}$$

Let us introduce another operator $a_{(-)}$, s.t.

$$a_{(-)}\psi_0 = 0$$

$a_{(-)}$: Step down Operator

$$a_{(-)}\psi_n = C_1\psi_{(n-1)}$$

$$\boxed{a_{(-)}|n\rangle = C_1|n-1\rangle} \qquad \boxed{C_1 = \sqrt{n}}$$

Correspondingly,

$$\boxed{a_{(+)}|n\rangle = C_2|n+1\rangle} \qquad \boxed{C_2 = \sqrt{n+1}}$$

$a_{(+)}$: Step up operator

$$\boxed{\begin{aligned} a_{(+)} &= (m\omega X - iP_x)\frac{1}{\sqrt{2\hbar m\omega}} \\ a_{(-)} &= (m\omega X + iP_x)\frac{1}{\sqrt{2\hbar m\omega}} \end{aligned}}$$

$$a_{(+)}a_{(-)} = \frac{1}{2\hbar m\omega}\Big((m\omega X - iP_x)(m\omega X + iP_x)\Big)$$

$$= \frac{1}{2\hbar m\omega}\left(m^2\omega^2 X^2 + im\omega(XP_x - P_xX) + P_x^2\right)$$

$$= \frac{1}{\hbar\omega}\left(\frac{P_x^2}{2m} + \frac{1}{2}m\omega^2X^2 + \frac{i\omega}{2}(i\hbar)\right)$$

$$= \frac{1}{\hbar\omega}\left(H - \frac{\hbar\omega}{2}\right)$$

$$\boxed{a_{(+)}a_{(-)} = \left(\frac{H}{\hbar\omega} - \frac{1}{2}\right)}$$

$\Rightarrow$ $a_{(+)}a_{(-)}$: Pure Number

$\Rightarrow$ $\hbar\omega\left(a_{(+)}a_{(-)} + \frac{1}{2}\right) = H$

Similarly

$$\boxed{a_{(-)}\, a_{(+)} = \frac{H}{\hbar\omega} + \frac{1}{2}}$$

$$\Rightarrow H = \hbar\omega\left(a_{(-)}\, a_{(+)} - \frac{1}{2}\right)$$

$$\Rightarrow \quad a_{(+)}\, a_{(-)} - a_{(-)}\, a_{(+)} = -1$$

$$\Rightarrow \quad \boxed{[a_{(+)}\ \ a_{(-)}] = -1}$$

Note that we can find X, P_x, H in terms of $a_{(+)}$ and $a_{(-)}$.

eg. $$X = \frac{\sqrt{2\hbar m\omega}}{2m\omega}\left(a_{(+)} + a_{(-)}\right)$$

$$= \sqrt{\frac{\hbar}{2m\omega}}\left(a_{(+)} + a_{(-)}\right)$$

$$P_x = \frac{\sqrt{2\hbar m\omega}}{2i}\left(a_{(-)} - a_{(+)}\right)$$

$$= i\sqrt{\frac{\hbar m\omega}{2}}\left(a_{(+)} - a_{(-)}\right)$$

define: ① a_+, a_-

② $N = a_+ a_-$ (define)

③ $|n\rangle$ as eigen functions of N with eigen value n. (a number)

④ $[N\ a_+] = a_+$
using $[a_+ a_-] = -1$
$[a_- a_+] = 1$

⑤ $[N\ a_-] = -a_-$

⑥ $N[a_+|n\rangle] = (n+1)|n\rangle$
$\Rightarrow a_+|n\rangle = c_1|n+1\rangle$

⑦ $N[a_-|n\rangle] = (n-1)\ a_-|n\rangle$
$\Rightarrow a_-|n\rangle = c_2|n-1\rangle$

⑧ using norm
$\langle n|a_- a_+|n\rangle = |c_1|^2$
$\langle n|N+1|n\rangle = |c_1|^2$
$|c_1| = \sqrt{n+1}$

⑨ $\langle n|a_+ a_-|n\rangle = |c_2|^2$
$|c_2| = \sqrt{n}$

⑩ $a_-|0\rangle = 0$

⑪ Prove $n \geq 0$
$n \in \mathbb{Z}$

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
$$\boxed{\begin{aligned}\langle T_n \rangle &= \left(n+\tfrac{1}{2}\right)\frac{\hbar\omega}{2} \\ \& \quad \langle V_n \rangle &= \left(n+\tfrac{1}{2}\right)\frac{\hbar\omega}{2}\end{aligned}}$$

$$\langle V_n \rangle = \frac{1}{2}m\omega^2 \langle x^2 \rangle$$

$$= \frac{1}{2}m\omega^2 \left| \psi_n \right| X^2 \left| \psi_n \right|$$

Now we can write X^2 in terms of $a_{(+)}$ and $a_{(-)}$

Similarly for K.E., we can write $E_n - \langle V_n \rangle = \langle T_n \rangle$

<u>To calculate E_0</u>

$$H\psi = E\psi$$

$$H_0\psi_0 = E_0\psi_0$$

$$\hbar\omega\,(a_{(-)}\,a_{(+)}\,\psi_0) - \frac{1}{2}\hbar\omega\,\psi_0$$

$$\hbar\omega\,(a_{(-)}\sqrt{1}\,\psi_1) - \frac{1}{2}\hbar\omega\,\psi_0$$

$$= \hbar\omega\left(\sqrt{1}\sqrt{1}.\ \psi_0\right) - \frac{1}{2}\hbar\omega\psi_0$$

$$= \frac{1}{2}\hbar\omega\psi_0$$

$$\Rightarrow \boxed{E_0 = \frac{1}{2}\hbar\omega}$$

To calculate ψ_0

Now $a_{(-)}\psi_0 = 0$

$$\Rightarrow \frac{1}{\sqrt{2\hbar m\omega}}\left(iP_x + m\omega X\right)\psi_0 = 0$$

$$\Rightarrow i\left(-i\hbar \frac{\partial \psi}{\partial x}\right) + m\omega x\psi_0 = 0$$

$$\Rightarrow \frac{\partial \psi_0}{\partial x} = -\left(\frac{m\omega x}{\hbar}\right)\psi_0$$

$$\Rightarrow \int \frac{d\psi_0}{d\psi_0} = -\frac{m\omega}{\hbar}\int x\, dx$$

$$\Rightarrow \boxed{\psi_0 = A e^{-\left(\frac{m\omega x^2}{2\hbar}\right)}}$$

$\langle \psi_0 | \psi_0 \rangle = 1$

$$\Rightarrow \boxed{A = \left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}}}$$

$a_+|\psi_0\rangle = |\psi_1\rangle$

$a_+|\psi_1\rangle = \sqrt{2}\,|\psi_2\rangle$

To find ψ_1

$$\Rightarrow \psi_1 = a_{(+)}|\psi_0\rangle$$

$$= \frac{1}{\sqrt{2\hbar m\omega}}\left[-iP_x + m\omega X\right]\left[\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} e^{-\frac{m\omega x^2}{2\hbar}}\right]$$

$$= \frac{2m\omega}{\sqrt{2\hbar m\omega}}\left(\frac{m\omega}{\pi\hbar}\right)^{\frac{1}{4}} x\, e^{-\left(\frac{m\omega x^2}{2\hbar}\right)}$$

$$H_1\psi_1 = E_1\psi_1$$

To find E_1

$$\hbar\omega\left(a_{(-)}a_{(+)} - \frac{1}{2}\right)\psi_1$$

$$= \hbar\omega\left(a_{(-)}a_{(+)}\psi_1 - \frac{1}{2}\psi_1\right)$$

$$= \hbar\omega\left(\sqrt{2}\sqrt{2}.\ \psi_1 - \frac{1}{2}\psi_1\right)$$

$$= \frac{3}{2}\hbar\omega\ \psi$$

$$\Rightarrow \boxed{E = \frac{3}{2}\hbar\omega}$$

Or write

$a_-a_+ = N+1$

$= \hbar\omega(N|n\rangle) + \hbar\omega|n\rangle - \frac{1}{2}\hbar\omega|n\rangle$

$\hbar\omega|n\rangle + \frac{\hbar\omega}{2}|n\rangle$

$\left(n+\frac{1}{2}\right)\hbar\omega|n\rangle$

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 !!

$$X = \sqrt{\frac{\hbar}{2m\omega}}\,(a_{(+)} + a_{(-)})$$

$$X^2 = \left(\sqrt{\frac{\hbar}{2m\omega}}\right)^2 (a_{(+)}^2 + a_{(-)}^2 + a_{(+)}a_{(-)} + a_{(-)}a_{(+)})$$

$$= \frac{\hbar}{2m\omega}\left(a_{(+)}^2 + a_{(-)}^2 + 2a_{(-)}a_{(+)} + 1 \right)$$

$$\langle n | x | n \rangle = \sqrt{\frac{\hbar}{2m\omega}} \langle n | a_{(+)} + a_{(-)} | n \rangle$$

$$= \sqrt{\frac{\hbar}{2m\omega}} \langle n | \sqrt{n+1}\, |n+1\rangle + \sqrt{\frac{\hbar}{2m\omega}} \langle n | \sqrt{n}\, |n-1\rangle$$

$$= 0 + 0$$

$$= 0$$

they will vanish

$$\langle n | x^2 | n \rangle$$

$$= \frac{\hbar}{2m\omega} \langle n | a_{(+)}^2 + a_{(-)}^2 + 2a_{(-)}a_{(+)} - 1 | n \rangle$$

$$= \frac{\hbar}{2m\omega} \langle n | 2a_{(-)}a_{(+)} - 1 | n \rangle$$

$$= \frac{\hbar}{m\omega} \langle n | a_{(-)}a_{(+)} | n \rangle - \frac{\hbar}{2m\omega} \langle n | n \rangle$$

$$= \frac{\hbar}{m\omega} \langle n | a_{(-)} \sqrt{n+1}\, |n+1\rangle - \frac{\hbar}{2m\omega} \langle n | n \rangle$$

$$= \frac{(\sqrt{n+1})^2 \hbar}{m\omega} \langle n | n \rangle - \frac{\hbar}{2m\omega} \langle n | n \rangle$$

$$= \left[(n+1) - \frac{1}{2} \right] \frac{\hbar}{m\omega}$$

$$= \left(n + \frac{1}{2} \right) \frac{\hbar}{m\omega}$$

$$\langle V \rangle = \frac{1}{2} m \omega^2 \langle x^2 \rangle$$

$$= \frac{1}{2} m \omega^2 (2n+1) \frac{\hbar}{2m\omega}$$

$$\boxed{\langle V_n \rangle = \frac{\hbar \omega}{2} \left(n + \frac{1}{2}\right)}$$

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 $0 < x < L$

$$\langle \psi | \psi \rangle = \frac{8}{L^3} \int_0^L \int_0^L \int_0^L \sin^2\left(\frac{\pi x}{L}\right) \sin^2\left(\frac{\pi y}{L}\right) \sin^2\left(\frac{\pi z}{L}\right) dx\, dy\, dz$$

$$= \frac{8}{L^3} \int \int \left(\frac{L}{2}\right) \sin^2\left(\frac{\pi y}{L}\right) \sin^2\left(\frac{\pi z}{L}\right) dy\, dz$$

$$= \frac{8}{L^3} \cdot \frac{L^3}{8} = 1$$

$$\langle p_x \rangle = \frac{\langle \psi | P_x | \psi \rangle}{\langle \psi | \psi \rangle} = \langle \psi | P_x | \psi \rangle$$

$$\langle p_x^2 \rangle = \frac{\langle \psi | P_x^2 | \psi \rangle}{\langle \psi | \psi \rangle} = \langle \psi | P_x^2 | \psi \rangle$$

$$\langle\psi|P_x|\psi\rangle = \langle\psi| -i\hbar\frac{\partial}{\partial x}\psi\rangle$$

$$= -i\hbar\iiint \psi^*(x,y,z)\ \frac{\partial\psi}{\partial x}\ dx\,dy\,dz$$

$$= -i\hbar\int_0^L\int_0^L\int_0^L \left(\frac{8}{L^3}\right)\sin\left(\frac{\pi x}{L}\right)\sin^2\left(\frac{\pi y}{L}\right)\sin^2\left(\frac{\pi z}{L}\right)\cos\left(\frac{\pi x}{L}\right) dx\,dy\,dz$$

$$= \frac{\pi}{L}\,\frac{-i\hbar 4}{L^3}\underbrace{\int_0^L \sin\frac{2\pi x}{L}\,dx}_{0}\ \int_0^L \sin^2\left(\frac{\pi y}{L}\right)dy\int_0^L \sin^2\left(\frac{\pi z}{L}\right)dz$$

$$= 0$$

⊙ 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)

$$\psi(x) = c_1\phi_1(x) + c_2\phi_2(x)$$

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

$$\psi(x) = c\sqrt{\frac{a}{2}}\sqrt{\frac{2}{a}}\sin\left(\frac{\pi x}{a}\right) + \frac{c}{2}\sqrt{\frac{a}{2}}\sqrt{\frac{2}{a}}\sin\left(\frac{2\pi x}{a}\right)$$

$$= c\sqrt{\frac{a}{2}}\,\phi_1(x) + \frac{c\sqrt{a}}{2\sqrt{2}}\,\phi_2(x)$$

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

$$c^2\frac{a}{2} + \frac{c^2 a}{8} = 1$$

$$c = \sqrt{\frac{8}{5a}}$$

★ 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 pure numbers.

$$\Rightarrow \psi(x) = \sqrt{\frac{8}{5a}}\sin\left(\frac{\pi x}{a}\right) + \sqrt{\frac{2}{5a}}\sin\left(\frac{2\pi x}{a}\right)$$

$$= \sqrt{\frac{4}{5}}\,\phi_1(x) + \sqrt{\frac{1}{5}}\,\phi_2(x)$$

$\langle E\rangle$

$$= \langle\psi|H|\psi\rangle$$

$$= \frac{4}{5}\langle\phi_1|H|\phi_1\rangle + \frac{1}{5}\langle\phi_2|H|\phi_2\rangle$$

$$\langle n|H|n\rangle = n^2\frac{h^2}{8ma^2}$$

$$\Rightarrow \frac{4}{5}\cdot\left(\frac{h^2}{8ma^2}\right) + \frac{1}{5}\cdot 4\left(\frac{h^2}{8ma^2}\right) = \frac{h^2}{5ma^2}$$

(★) $P_i = |C_i|^2 = |\langle \phi_i | \psi \rangle|^2$ if $\psi = \sum C_i \phi_i$

Q An e^- is given in $|l, m\rangle = \frac{1}{\sqrt{14}} Y_3^0 + \frac{2}{\sqrt{14}} \cdot Y_3^{-1} + \frac{3}{\sqrt{14}} Y_2^2$

Find $\langle L^2 \rangle$, $\langle L_z \rangle$
$\langle S_z \rangle$ $\langle S_z^2 \rangle$ $\langle \mu_z \rangle$

We can see $\langle l, m | l, m \rangle = 1$

$$\langle l, m | L^2 | l, m \rangle = l(l+1)\hbar^2$$

$$\langle l, m | L_z | l, m \rangle = m_l \hbar$$

$$\langle l, m | L^2 | l, m \rangle = \frac{1}{14} \langle 3,0 | L^2 | 3,0 \rangle$$ 12

$$+$$

$$\frac{4}{14} \langle 3,-1 | L^2 | 3,-1 \rangle$$ 48

$$+$$

$$\frac{9}{14} \langle 2,2 | L^2 | 2,2 \rangle$$ 54

$$= \left(\frac{104}{14}\right) \hbar^2$$

$$\langle l, m | L_z | l, m \rangle$$

$$= \frac{1}{14} \cdot 0 + \frac{4}{14} \cdot (-1\hbar) + \frac{9}{14} (2\hbar)$$

$$= \hbar$$

$$\boxed{\begin{aligned} \vec{\mu} &= \vec{\mu}_L + \vec{\mu}_s \\ &= \frac{-e}{2m} (\vec{L} + 2\vec{S}) \end{aligned}}$$

$$\mu_z = \frac{-e}{2m} (L_z + 2S_z)$$

$$\langle \mu_z \rangle = \frac{-e}{2m} (\langle L_z \rangle + 2 \langle S_z \rangle)$$

$$= -\frac{e\hbar}{2m} + \frac{e}{m} \langle S_z \rangle$$

$$S_z = m_s \hbar = \pm \frac{1}{2} \hbar$$

$$\langle S_z \rangle = \langle s, m | S_z | s, m \rangle$$

Wave Function has no relation with spin.

$$= \langle \chi_+ | S_z | \chi_- \rangle + \langle \chi_- | S_z | \chi_- \rangle$$

$$|s, m\rangle = c_1 \chi_{(+)} + c_2 \chi_{(-)}$$

(if given)

$$\chi = \begin{pmatrix} -\frac{3i}{5} \\ 4 \end{pmatrix}$$

$$\langle S_z \rangle = |c_1|^2 \langle \chi_+ | S_z | \chi_+ \rangle + |c_2|^2 \langle \chi_- | S_z | \chi_+ \rangle$$

$$= \frac{9}{25} \langle \chi_+ | S_z | \chi_+ \rangle + \frac{16}{25} \langle \chi_- | S_z | \chi_- \rangle$$

$$= \frac{9}{25}\frac{1}{2}\hbar \begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

$$= \frac{1}{2}\hbar \; \frac{9}{25} \begin{bmatrix} 1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix}$$

$$= \frac{1}{2}\hbar \left(\frac{9}{25}\right)$$

$$+$$

$$\frac{1}{2}\hbar \frac{16}{25} \begin{bmatrix} 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

$$= \frac{\hbar 8}{25} \begin{bmatrix} 0 & -1 \end{bmatrix} \begin{bmatrix} 0 \\ 1 \end{bmatrix}$$

$$= -\frac{\hbar 8}{25}$$

$$\langle S_z \rangle = \frac{-7}{50}\hbar$$

Proof of H atom

Step 1 : Complete Equation

$$\frac{1}{r^2}\left(\frac{d}{dr}r^2\frac{d\psi}{dr}\right)+\frac{1}{r^2\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\psi}{d\theta}\right)$$

$$+\frac{1}{r^2\sin^2\theta}\frac{d^2\psi}{d\phi^2}+\frac{2m}{\hbar^2}\left(E+\frac{e^2}{4\pi\varepsilon_0 r}\right)\psi=0$$

Step 2 : Separate Φ by multiply by $r^2\sin^2\theta$ and writing ψ as $R\Theta\Phi$ and dividing by $R\Theta\Phi$

$$\frac{\sin^2\theta}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{\sin\theta}{\Theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)$$

$$+\frac{2mr^2}{\hbar^2}\left(E+\frac{e^2}{4\pi\varepsilon_0 r}\right)\sin^2\theta=-\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2}=m^2 \text{ (say)}$$

$$\boxed{\Phi=Ae^{im\phi}}$$

Step 3 : Separate Θ by dividing by $\sin^2\theta$

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{2m}{\hbar^2}r^2\left(E+\frac{e^2}{4\pi\varepsilon_0 r}\right)$$

$$=\left[\frac{m^2}{\sin^2\theta}-\frac{1}{\sin\theta\,\Theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)\right]$$

$$=l(l+1)\quad\text{(say)}$$

$$\boxed{\Theta=P_l^m(\cos\theta)}$$

$\Rightarrow$

Step 4 : Write the "r" equation properly by multiplying by R and dividing by r^2

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\left[\frac{2mE}{\hbar^2}+\frac{2me^2}{4\pi\varepsilon_0\hbar^2 r}-\frac{l(l+1)}{r^2}\right]R=0$$

Step 5 : Substitution

Let

$\rho=2kr$ (dimensionless)

$k=\sqrt{\frac{-2mE}{\hbar^2}}$ (wave number)

$\lambda=\left(\frac{me^2}{4\pi\varepsilon_0\hbar^2 k}\right)$ (dimensionless)

replacing and dividing by $4k^2$,

$$\frac{1}{\rho^2}\frac{d}{d\rho}\left(\rho^2\frac{dR}{d\rho}\right)+\left[-\frac{1}{4}+\frac{\lambda}{\rho}-\frac{l(l+1)}{\rho^2}\right]=0$$

Step 6 : Assymptotic behaviour

When $\rho\to\infty$, i.e. $r\to\infty$, we have

$$\frac{1}{\rho^2}\frac{d}{d\rho}\left(\rho^2\frac{dR}{d\rho}\right)-\frac{R}{4}=0$$

We'll get $\boxed{R=e^{-\frac{\rho}{2}}}$

Step 7 : Polynomial function

Let the solution be of form

$R=e^{-\frac{\rho}{2}}F(\rho)$

where F is a polynomial

$$\Rightarrow\frac{dR}{d\rho}=-\frac{1}{2}e^{-\frac{\rho}{2}}F+e^{-\frac{\rho}{2}}F'$$

$$\Rightarrow\frac{1}{\rho^2}\frac{d}{d\rho}\left(\rho^2\frac{dR}{d\rho}\right)=e^{-\frac{\rho}{2}}F''+\left(\frac{2}{\rho}-1\right)e^{-\frac{\rho}{2}}F'+\left(\frac{1}{4}-\frac{1}{\rho}\right)e^{-\frac{\rho}{2}}F$$

Using it in the actual equation,

$$e^{-\frac{\rho}{2}}\Big[\rho F'' + F'\left[\frac{2}{\rho}-1\right] + F\left[\frac{1}{4}-\frac{1}{\rho}\right] + \left[\frac{-1}{4}+\frac{\lambda}{\rho}-\frac{l(l+1)}{\rho^2}\right]F\Big] = 0$$

$$\Rightarrow \quad F'' + F'\left[\frac{2}{\rho}-1\right] + F\left[\frac{\lambda-1}{\rho}-\frac{l(l+1)}{\rho^2}\right] = 0$$

<u>Step 8</u> <u>Use power series to expand</u>

let $F(\rho) = \rho^s \sum_{j=0} a_j \rho^j = \rho^s G(\rho)$

where $j, s \in \mathbb{Z}^+$ (positive integers)

Otherwise at $\rho=0$, $F\to\infty$

This form ensures that F is finite at $\rho = 0$

$$\Rightarrow \sum a_j \{(j+s)(j+s+1) - l(l+1)\}\rho^{j+s-2} - \sum a_j\{(j+s) - (\lambda-1)\}\rho^{s+j-1} = 0$$

<u>Step 9</u> <u>Separating $j=0$ from 1st term</u>

$$\Rightarrow a_0\{s(s+1) - l(l+1)\}\rho^{s-2} + \sum_{j=1} a_j\{(j+s)(j+s+1) - l(l+1)\}\rho^{j+s-2} - \sum_{j=0} a_j\{(j+s) - (\lambda-1)\}\rho^{j+s-1} = 0$$

Put $j = j'+1$

$$\Rightarrow a_0\{s(s+1) - l(l+1)\}\rho^{s-2} + \sum_{j'=0} a_{j'+1}\{(j'+s+1)(j'+s+2) - l(l+1)\}\rho^{j'+s-1} - \sum_{j=0} a_j\{(j+s) - (\lambda-1)\}\rho^{j+s-1} = 0$$

Replacing j' by j as its just a symbol for summation, we have

$$a_0(s(s+1) - l(l+1))\rho^{s-2} + \sum_j \Big(a_{j+1}\left[(j+s+1)(j+s+2) - l(l+1)\right] - a_j\left[(j+s) - (\lambda-1)\right]\Big)\rho^{s+j-1} = 0$$

<u>Step 10</u> <u>Putting Coefficient $=0$</u>

If $A + Bx + Cx^2 = 0$ for all x

$\Rightarrow A = B = C = 0$

$\therefore$ we have

$s(s+1) - l(l+1) = 0$

$\Rightarrow s = l$ or $s = -(l+1)$

$\Rightarrow \boxed{s = l}$ $\quad s \in \mathbb{Z}^+$

$$[(j+s+1)(j+s+2) - \ell(\ell+1)]\, a_{j+1} - a_j[(j+s) - (\lambda-1)] = 0$$

$$\Rightarrow \frac{a_{j+1}}{a_j} = \frac{(j+\ell) - (\lambda-1)}{(j+\ell+1)(j+\ell+2) - \ell(\ell+1)}$$

Step 11 Termination/ Truncation for some power of j

$$j_{max} + \ell - \lambda + 1 = 0$$

$$\Rightarrow \lambda = j_{max} + \ell + 1 = n \text{ (say)}$$

$$\therefore n \in \mathbb{Z} \Rightarrow \lambda \in \mathbb{Z}$$

$$\Rightarrow \lambda = \ell+1,\ \ell+2,\ \ell+3,\ \dots = n$$

Now $\lambda = \frac{me^2}{4\pi\varepsilon_0 \hbar^2 k}$ and $k = \sqrt{\frac{-2mE}{\hbar^2}}$

$$\Rightarrow n^2 = -\frac{m^2 e^4}{(4\pi\varepsilon_0)^2 \hbar^2} \frac{\hbar^2}{2mE}$$

$$\Rightarrow \boxed{E = -\frac{me^4}{2(4\pi\varepsilon_0)^2 \hbar^2 n^2}}$$

$$= -\left(\frac{13.6}{n^2}\right) eV$$

Step 12 Eigen Function

Put $F = \rho^\ell G(\rho)$, we get

$$F'' = \rho^\ell G'' + 2\ell\rho^{\ell-1} G' + \ell(\ell-1)\rho^{\ell-2}G$$

$$F'\left(\frac{2}{\rho} - 1\right) = G'(2\rho^{\ell-1} - \rho^\ell) + G(2\ell\rho^{\ell-2} - \ell\rho^{\ell-1})$$

$$F\left[\frac{\lambda-1}{\rho} - \frac{\ell(\ell+1)}{\rho^2}\right] = G[(\lambda-1)\rho^{\ell-1} - \ell(\ell+1)\rho^{\ell-2}]$$

Step 13 divide by $\rho^{\ell-1}$ and combine $(2\ell+1)$, we get

$$\rho G'' + ((2\ell+1) + 1 - \rho) G' + [(n+\ell) - (2\ell+1)] G = 0$$

This is precisely the Associated Laguerre Equation, whose solution is

$$G(\rho) = C\, L^{2\ell+1}_{n+\ell}(\rho)$$

where $L^{2\ell+1}_{n+\ell} = \frac{d^{2\ell+1}}{d\rho^{2\ell+1}}(L_{n+\ell})$

is called Associated Laguerre Polynomial

& $L_n(\rho) = e^\rho \frac{d^n}{d\rho^n}(\rho^n e^{-\rho})$

Step 14 Replace ρ

Now $\rho = \left(\dfrac{2Zr}{na_0}\right)$

where $a_0 =$ bohr's radius

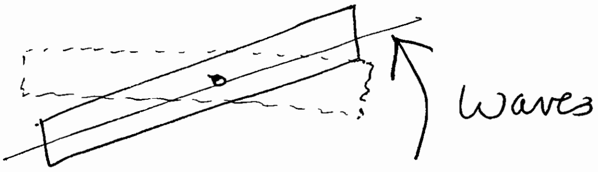
$= \left(\dfrac{4\pi\varepsilon_0 \hbar^2}{me^2}\right)$

$$\Rightarrow \boxed{R(\rho) = C\, e^{-\left(\frac{\rho}{2}\right)} \rho^{l} L_{n+l}^{2l+1}(\rho)}$$

$$\boxed{= C\, e^{-\frac{Zr}{na_0}} \left(\frac{2Zr}{na_0}\right)^{l} L_{n+l}^{2l+1}\left(\frac{2Zr}{na_0}\right)}$$

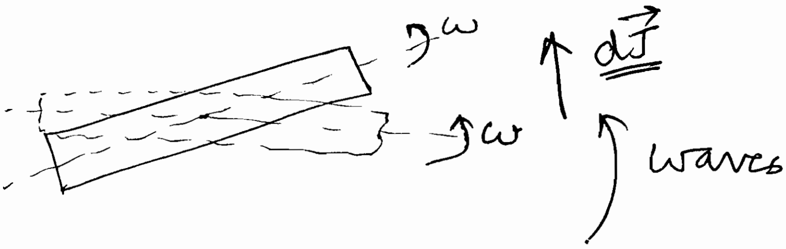
For $n =$ [redacted], $l = 0$, $m = 0$

$$\psi_{1} = \frac{1}{\sqrt{\pi}} \left(\frac{Z}{a_0}\right)^{\frac{3}{2}} e^{-\frac{Zr}{a_0}}$$



easily disbalanced

but if



waves cannot provide marked $d\vec{J}$ in that direction. Hence stable

⇒ Similarly

bullet motion spiral type due to groves 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.

- P-49 Ans: $\sqrt{\frac{2V_0 a^2}{m}}$

Method-1 $\sqrt{\frac{1}{m}\left(\frac{d^2V}{dx^2}\right)}$

Method-2 Open $V(r)$ in form of Taylor expansion, ignore higher power of $(r-r_0)$

- P-54 : (1)

- P 88
- P-90
- P-97
- P-98
- P-168
- P-12 (II) <u>14</u> (Bound states)
- P-78